Spectral theory for generalized bounded variation perturbations of orthogonal polynomials and Schrödinger operators

Thesis by

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To my parents

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Abstract

The purpose of this text is to present some new results in the spectral theory of orthogonal polynomials and Schrödinger operators.

These results concern perturbations of the free Schrödinger operator $-\Delta$ and of the free case for orthogonal polynomials on the unit circle (which corresponds to Verblunsky coefficients $\alpha_n \equiv 0$) and the real line (which corresponds to off-diagonal Jacobi coefficients $a_n \equiv 1$ and diagonal Jacobi coefficients $b_n \equiv 0$).

The condition central to our results is that of generalized bounded variation. This class consists of finite linear combinations

$$V(x) = \sum_{l=1}^{L} \beta_l(x) + W(x)$$

where $e^{i\phi_l x}\beta_l(x)$ has bounded variation with some phase ϕ_l and $W \in L^1$. This generalizes both usual bounded variation and expressions of the form

$$\lambda(x)\cos(\phi x + \alpha)$$

with $\lambda(x)$ of bounded variation (and, in particular, with $\lambda(x) = x^{-\gamma}$, Wigner–von Neumann potentials) as well as their finite linear combinations.

Assuming generalized bounded variation and an L^p condition (with any $p < \infty$) on the perturbation, our results show preservation of absolutely continuous spectrum, absence of singular continuous spectrum, and that embedded pure points in the continuous spectrum can only occur in an explicit finite set.

Contents

Introduction

The purpose of this text is to present some new results in the spectral theory of orthogonal polynomials and Schrödinger operators. The statements of these results are given in Section 4.2; Section 4.1 contains a discussion of related results which served as motivation for our work, and the remainder of Chapter 4 contains the proof of our results.

Throughout this text, we assume that the reader has a certain level of knowledge in analysis. More specifically, we will assume knowledge of topics such as measure theory, Banach and Hilbert spaces. Although prior exposure to spectral theory would certainly help the reader to put the results in perspective, we will not assume it.

Chapters 1–3 of this text are expository and cover the necessary prerequisites in spectral theory. Chapter 1 will introduce some basic notions of spectral theory, Chapter 2 the basics of orthogonal polynomials, and Chapter 3 the basics of Schrödinger operators. Our goal was to provide the background needed for our results in a limited amount of space, so our choice of topics in Chapters 1–3 is very biased and we make no effort to provide a more general review of spectral theory. For more information, we refer the reader to books on the subject, such as those by Reed–Simon [49, 50, 51, 52], Simon [60, 61, 63], and Teschl [71, 72].

Chapter 1

Linear operators on Hilbert spaces

1.1 Introduction

In this chapter we will present some basic notions about linear operators on Hilbert spaces. Our main goal is to establish the basic facts about unitary and self-adjoint operators, which will be needed in the remainder of this text. In particular, we will discuss unbounded self-adjoint operators, which will be needed for our discussion of Schrödinger operators in Chapter 3. Our exposition will focus on unbounded operators from the start, since the theory we present includes bounded operators as a special case.

We assume that the reader has already encountered Hilbert spaces and is familiar with basic Hilbert space theory as explained in most functional analysis textbooks, for example, in [49, Chapter 2] or [57, Chapter 4]. We will not repeat these definitions, but we will stress a notational choice: in this text, we define the inner product $\langle f, g\rangle$ to be linear in the second parameter and conjugate-linear in the first parameter. Both this and the alternative convention (that the inner product be linear in the first parameter and conjugate-linear in the second) are common in the literature, and the difference is clearly only notational, since it can be fixed by switching the two parameters. Consistent with this convention, we consider any space of square-integrable functions, $L^2(X, d\mu)$, a Hilbert space with the inner product

$$\langle f, g\rangle = \int \bar{f} g d\mu$$

After the construction of the Lebesgue integral, the space $L^2(a, b)$ of square-integrable functions on an interval was used to analyze Fourier series and other orthogonal expansions. In particular, Riesz [53] and Fischer [19] proved in 1907 that $L^2(a, b)$ is complete and thus isomorphic to $\ell^2(\mathbb{N})$, and Fredholm's work on integral equations [20] in 1903 used orthogonal expansions and the concept of an adjoint equation to analyze eigenvalue problems for integral operators. The basics of Hilbert space theory were developed in the early 20th century by Hilbert and his school, especially Schmidt and von Neumann. The spectral theorem for bounded self-adjoint operators was proved by Hilbert [30], with contributions by Riesz [54]. The extension to unitary operators and unbounded self-adjoint operators is due to von Neumann [74].

1.2 Unbounded operators and adjoints

The mathematical theory of unbounded operators was developed in the 1930s by von Neumann [74] and Stone [67]. With the development of quantum physics in the early 20th century, it quickly became clear that in a mathematical theory of quantum physics, experimentally observable quantities have to be represented, in general, by non-commuting objects rather than scalars, and it was ultimately recognized that unbounded operators are the proper framework for a rigorous mathematical foundation for quantum mechanics.

To develop some motivation for unbounded operators, we will first informally discuss two examples. As the first example, assume that we wish to define an operator

$$T\colon f(x) \mapsto xf(x)$$

acting on complex-valued functions on $\mathbb{R}$. This is a well-defined linear operator on the set of all measurable functions, but what if we wish to restrict it to an operator on $L^2(\mathbb{R})$? We would have to restrict T to the smaller domain, $D(T)$, of functions for which $xf(x)$ is in $L^2(\mathbb{R})$:

$$D(T) = \{f(x) \in L^2(\mathbb{R}) \mid xf(x) \in L^2(\mathbb{R})\}$$

Although $D(T) \subsetneq L^2(\mathbb{R})$, one can see that $D(T)$ contains all functions of bounded support (since $\int |xf(x)|^2 dx \leq M^2 \int |f(x)|^2 dx$ if $\operatorname{supp} f \subset [-M, M]$), so $D(T)$ is a dense subset of $L^2(\mathbb{R})$. Similarly, note that if $f \in D(T)$ with $\operatorname{supp} f \subset [M, 2M]$, then $\|Tf\|_2 \geq M\|f\|_2$, so T is not a bounded operator from $D(T)$ to $L^2(\mathbb{R})$. Thus, there are two peculiarities about this operator: its domain is not all of $L^2(\mathbb{R})$ and it is not bounded.

As the second example, assume that we want to make the Laplacian Δ into an operator on $L^2(\mathbb{R}^n)$. It is clear that not every $f \in L^2(\mathbb{R}^n)$ is twice differentiable, but we may try to fix that by allowing weak derivatives (in the sense of tempered distributions). However, the weak derivatives are, in general, distributions and need not be functions, let alone square-integrable. It is thus clear that we will have to resign to defining Δ only on a domain $D(\Delta)$ which is a subset of $L^2(\mathbb{R}^n)$. On the other hand, we probably want $D(\Delta)$ to include at least $C_0^\infty(\mathbb{R}^n)$, the set of infinitely differentiable functions with compact support. By constructing rapidly oscillating C_0^∞ functions, it is easy to see that Δ has no chance of being a bounded operator. We thus need a proper framework for operators which are unbounded and not everywhere defined. We must also address the concern of whether our choice of domain affects properties of the operator, and we will see that it sometimes does. For example, for differential operators, boundary conditions often get encoded into the domain.

In carrying over the theory of bounded operators to unbounded, not everywhere defined operators, some care is needed. Some notions carry over by obvious analogy from the bounded operator case; for example, one can still discuss eigenvalues and eigenfunctions of T, with the obvious caveat that eigenfunctions must be elements of $D(T)$. But for other notions, one must be more careful; for example, one might (wrongly!) think that the analogue of self-adjointness is

$$\langle g, Tf\rangle = \langle Tg, f\rangle, \quad \forall f, g \in D(T) \tag{1.2.1}$$

In fact, operators obeying (1.2.1) are called symmetric operators, a notion weaker than self-adjointness. The difference between these two notions will be discussed in Section 1.3, and a motivation for the stronger definition of self-adjointness will be provided by the spectral theorem for self-adjoint operators (Theorem 1.8.1).

Complications can arise for notions as simple as composition of operators. For unbounded A, B, we can only define AB on $D(AB) = \{f \in D(B) \mid Bf \in D(A)\}$, but there is no guarantee that $D(AB)$ is dense in $L^2(\mathbb{R})$ or even different than $\{0\}$.

For yet other concepts, there is no obvious way to generalize them, although it can be done. For a bounded operator T, it is customary to define functions of T by power series; for example, the operator $\exp(itT)$ is customarily defined by a power series,

$$e^{itT} f = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} T^n f \tag{1.2.2}$$

If T is bounded, it is easy to check that the power series converges for every f, but for an unbounded operator we have to explain what we mean by T^n, the sum only makes sense for $f \in \cap_{n=0}^{\infty} D(T^n)$, and even then convergence of the series is an issue. We will see in Section 1.9 that there is a better way to establish functional calculus of operators, at least in the self-adjoint case.

Definition 1.2.1. An *unbounded operator* A on a Hilbert space $\mathcal{H}$ is a linear map $A\colon D(A) \to \mathcal{H}$ defined on a linear subspace $D(A) \subset \mathcal{H}$. We will also always assume that $D(A)$ is dense in $\mathcal{H}$.

One of the main difficulties in dealing with unbounded operators is in the need to be careful about domains. It should not be surprising then that some bounded operators associated with A will play an important role.

Definition 1.2.2. Let A be an unbounded operator on $\mathcal{H}$. The *resolvent* of A at $\lambda \in \mathbb{C}$, if it exists, is a bounded two-sided inverse of $A-\lambda$, denoted $R_\lambda(A)$, i.e. $R_\lambda(A)\colon \mathcal{H}\to D(A)$ is such that

$$R_\lambda(A)(A-\lambda)v = v, \quad \forall v\in D(A)$$
$$(A-\lambda)R_\lambda(A)v = v, \quad \forall v\in \mathcal{H}$$

The *spectrum* of A, denoted $\sigma(A)$, is the set of $\lambda\in\mathbb{C}$ for which the resolvent doesn't exist.

Remark 1.2.1. We warn the reader that some books define the resolvent as the inverse of $\lambda - A$, differing by a minus sign from our convention.

Remark 1.2.2. Uniqueness of $R_\lambda(A)$, if it exists, follows from a standard algebraic argument: if $\tilde{R}_\lambda(A)$ also satisfies all the properties, then $R_\lambda(A) = R_\lambda(A)(A-\lambda)\tilde{R}_\lambda(A) = \tilde{R}_\lambda(A)$.

The following theorem establishes some properties of the resolvent and shows that the spectrum is a closed set.

Theorem 1.2.1. *(i) (The first resolvent identity) For any $z, w\notin\sigma(A)$,*

$$R_z(A) - R_w(A) = (z-w)R_z(A)R_w(A) \tag{1.2.3}$$

(ii) For any $z, w\notin\sigma(A)$, $R_z(A)R_w(A) = R_w(A)R_z(A)$.

(iii) $\sigma(A)$ is closed and the map $\lambda\mapsto R_\lambda(A)$ is a norm-analytic map of $\mathbb{C}\setminus\sigma(A)$ to $\mathcal{B}(\mathcal{H})$.

We remind the reader that a norm-analytic map from a region $\Omega\subset\mathbb{C}$ to $\mathcal{B}(\mathcal{H})$ is a map which is representable by a norm-convergent power series in a neighborhood of any point of Ω.

Proof. (i) follows from the calculation

$$R_z(A)(z-w)R_w(A) = R_z(A)[(A-w)-(A-z)]R_w(A) = R_z(A) - R_w(A)$$

(ii) follows from (i) by interchanging z and w and comparing the two equalities.

To prove (iii), fix $z\notin\sigma(A)$ and let $r = \|R_z(A)\|^{-1}$. Define

$$\hat{R}_w(A) = \sum_{n=0}^{\infty}(w-z)^n R_z(A)^{n+1} \tag{1.2.4}$$

This clearly defines a norm-analytic function of w in the disk $|w-z|<r$, and a straightforward calculation shows that $\hat{R}_w(A)(A-w) = (A-w)\hat{R}_w(A) = 1$, so $w\notin\sigma(A)$ and in the disk $|w-z|<r$, the resolvent is given by the norm-analytic power series (1.2.4). □

The spectrum of a matrix is just its set of eigenvalues. For an operator A on an infinite-dimensional space, if λ is an eigenvalue, then $\operatorname{Ker}(A-\lambda)\neq\{0\}$ so $\lambda\in\sigma(A)$, but the converse does not hold: elements of $\sigma(A)$ are not necessarily eigenvalues, as seen in the following example.

Example 1.2.1. Let A be a bounded operator on $L^2(0,1)$ given by $(Af)(x) = xf(x)$. For $z \in \mathbb{C}\backslash[0,1]$, multiplication by $(x-z)^{-1}$ is a bounded inverse for $A - z$, so $z \notin \sigma(A)$. For $z \in [0,1]$, picking a function $f \in L^2(0,1)$ with $\operatorname{supp} f \subset [z-\epsilon, z+\epsilon]$, we have $\|(A-z)f\|_2 \le \epsilon \|f\|_2$, so $A - z$ cannot have a bounded inverse. Thus, $\sigma(A) = [0,1]$. However, $Af = zf$ implies that $xf(x) = zf(x)$ for a.e. x, so $f = 0$. Thus, A has no eigenvalues.

We now introduce the graph of an unbounded operator and some related properties. The usefulness of graphs in the study of unbounded operators was first shown by von Neumann [75]. We will use the Hilbert space structure on $\mathcal{H} \times \mathcal{H}$, given by the inner product

$$\langle (u_1, v_1), (u_2, v_2) \rangle = \langle u_1, u_2 \rangle + \langle v_1, v_2 \rangle \tag{1.2.5}$$

Definition 1.2.3. (i) The *graph* of an operator A on $\mathcal{H}$ is

$$\Gamma(A) = \{(u, Au) \in \mathcal{H} \times \mathcal{H} \mid u \in D(A)\} \tag{1.2.6}$$

(ii) An *extension* of A is an operator B such that $\Gamma(A) \subset \Gamma(B)$.

(iii) An operator A is *closed* in $\mathcal{H}$ if and only if $\Gamma(A)$ is closed in $\mathcal{H} \times \mathcal{H}$.

(iv) A is *closable* if and only if it has a closed extension.

(v) If A is closable, its smallest closed extension is called its *closure* and denoted $\bar{A}$.

(vi) If A is closed, D is a *core* for A if and only if $\overline{A|_D} = A$.

Remark 1.2.3. If A is closable, the intersection of all its closed extensions (more precisely, the operator corresponding to the intersection of graphs of all its closed extensions) is its smallest closed extension.

Definition 1.2.4. An bounded operator $U\colon \mathcal{H} \to \mathcal{K}$ is *unitary* if and only if $\operatorname{Ran} U = \mathcal{K}$ and $\|Uv\| = \|v\|$ for all $v \in \mathcal{H}$.

Remark 1.2.4. By the polarization identity

$$\langle u, v \rangle = \tfrac{1}{4}\left(\|u+v\|^2 - \|u-v\|^2 + i\|u+iv\|^2 - i\|u-iv\|^2\right)$$

this is equivalent to the condition that $\operatorname{Ran} U = \mathcal{K}$ and $\langle Uu, Uv \rangle = \langle u, v \rangle$ for all $u, v \in \mathcal{H}$.

Let A be an unbounded operator on $\mathcal{H}$. We wish to define its adjoint A^*. For bounded operators, the adjoint is defined by the condition that

$$\langle A^* u, v \rangle = \langle u, Av \rangle \tag{1.2.7}$$

holds for all $u, v \in \mathcal{H}$, which determines A^* uniquely by the Riesz representation theorem. For unbounded operators, (1.2.7) is clearly only defined for $v \in D(A)$, but that is not the only modification needed: the left-hand side of (1.2.7) is a bounded linear functional in v, so the right-hand side must be as well. Conversely, if the right-hand side is a bounded linear functional on $D(A)$, then density of $D(A)$ and the Riesz representation theorem imply that the value of A^*u is uniquely determined by (1.2.7). Thus, we define

Definition 1.2.5. For an unbounded densely defined operator A on $\mathcal{H}$, define its adjoint A^* by

$$D(A^*) = \{u \in \mathcal{H} \mid \text{the map } v \mapsto \langle u, Av \rangle \text{ is a bounded map from } D(A) \text{ to } \mathbb{C}\} \tag{1.2.8}$$

and

$$\langle A^*u, v \rangle = \langle u, Av \rangle, \quad \forall u \in D(A^*)\ \forall v \in D(A) \tag{1.2.9}$$

Note that the fact that $D(A)$ is dense in $\mathcal{H}$ is what guarantees that A^*u is uniquely determined by (1.2.9). Using this uniqueness, the reader can easily verify that A^* is linear. We warn the reader that A^* isn't necessarily densely defined, so, for example, the double adjoint A^{**} may not be defined.

To establish some properties of the adjoint, we will use a unitary operator V on $\mathcal{H} \times \mathcal{H}$, defined by

$$V(\phi, \psi) = (-\psi, \phi) \tag{1.2.10}$$

Theorem 1.2.2. *Let A be an unbounded, densely defined operator.*

(i) The graph of the adjoint of A is given by

$$\Gamma(A^*) = V(\Gamma(A))^{\perp} \tag{1.2.11}$$

In particular, A^* is closed.

(ii) The kernel of the adjoint of A is given by

$$\operatorname{Ker} A^* = (\operatorname{Ran} A)^{\perp} \tag{1.2.12}$$

(iii) A is closable if and only if

$$\{\psi \mid (0, \psi) \in \overline{\Gamma(A)}\} = \{0\} \tag{1.2.13}$$

i.e. if and only if $\overline{\Gamma(A)}$ is the graph of an operator, in which case $\Gamma(\bar{A}) = \overline{\Gamma(A)}$.

(iv) A is closable if and only if $D(A^*)$ is dense, in which case $\bar{A} = A^{**}$.

(v) If A is closable, then $(\bar{A})^* = A^*$.

(vi) If $A \subset B$, then $B^* \subset A^*$.

Proof. (i) By rewriting (1.2.9) in terms of the inner product (1.2.5) on $\mathcal{H} \times \mathcal{H}$, we see $(\phi, \psi) \in \Gamma(A^*)$ is equivalent to $(\phi, \psi) \perp (-Au, u)$ for all $u \in D(A)$, so $\Gamma(A^*) = V(\Gamma(A))^\perp$.

(ii) This is immediate from (1.2.9).

(iii) Since $\overline{\Gamma(A)}$ is a linear subspace of $\mathcal{H} \times \mathcal{H}$, it is the graph of some operator B if and only if (1.2.13) holds. If so, then B is a closed extension of A, so A is closable and $\Gamma(\overline{A}) \subset \overline{\Gamma(A)}$.

Conversely, if A is closable, then since $\Gamma(\overline{A})$ is closed, $\Gamma(A) \subset \Gamma(\overline{A})$ implies $\overline{\Gamma(A)} \subset \Gamma(\overline{A})$. This and the criterion (1.2.13) imply that $\overline{\Gamma(A)}$ is the graph of an operator, and then using the previous paragraph, we conclude $\Gamma(\overline{A}) = \overline{\Gamma(A)}$.

(iv) Note that the proof of (i), applied to A^*, implies that $V\Gamma(A^*)^\perp$ is the set of vectors (ϕ, ψ) such that $\langle \psi, v \rangle = \langle \phi, A^* v \rangle$ for all $v \in D(A^*)$. This set of vectors is the graph of an operator if and only if ϕ uniquely determines ψ, i.e. if and only if $D(A^*)$ is dense. However, $V^2 = -1$ implies $V(\Gamma(A^*))^\perp = V(V\Gamma(A)^\perp)^\perp = \overline{\Gamma(A)}$, so $D(A^*)$ is dense if and only if $\overline{\Gamma(A)}$ is the graph of an operator, and in that case $\overline{\Gamma(A)} = \Gamma(A^{**})$.

(v) If A is closable, then by (iii) and (iii), $(\bar{A})^* = A^{***} = \overline{A^*} = A^*$.

(vi) $\Gamma(A) \subset \Gamma(B)$ implies $\Gamma(B^*) = V(\Gamma(B))^\perp \subset V(\Gamma(A))^\perp = \Gamma(A^*)$. □

1.3 Self-adjointness

In this section we discuss self-adjointness and related notions. We begin with a definition.

Definition 1.3.1. (i) An operator A is *symmetric* if

$$\langle Au, v \rangle = \langle u, Av \rangle, \quad \forall u, v \in D(A)$$

(ii) A is *essentially self-adjoint* if $\bar{A} = A^*$.

(iii) A is *self-adjoint* if $A = A^*$.

The property that A is symmetric is equivalent to $D(A) \subset D(A^*)$ and $A^*|_{D(A)} = A$, so every self-adjoint operator is symmetric. We will later see that the converse is false. Criteria for self-adjointness are of great interest, and here we present the most basic one.

Theorem 1.3.1. *For a symmetric operator A on $\mathcal{H}$, the following are equivalent:*

(i) A is self-adjoint.

(ii) A is closed and $\mathrm{Ker}(A^* \pm i) = \{0\}$.

(iii) $\mathrm{Ran}(A \pm i) = \mathcal{H}$.

For the proof, we will need an important inequality.

Lemma 1.3.2. *Let A be a symmetric operator, $\psi \in D(A)$, $z \in \mathbb{C} \setminus \mathbb{R}$. Then*

$$\|(A-z)\psi\| \geq |\operatorname{Im} z| \|\psi\| \tag{1.3.1}$$

Proof. Let $z = x + iy$, $x, y \in \mathbb{R}$. Then (1.3.1) is immediate from the calculation

$$\begin{aligned}\|(A-z)\psi\|^2 &= \langle (A-x-iy)\psi, (A-x-iy)\psi\rangle \\ &= \langle (A-x)\psi, (A-x)\psi\rangle - iy\langle (A-x)\psi, \psi\rangle + iy\langle \psi, (A-x)\psi\rangle + (-iy)(iy)\langle \psi, \psi\rangle \\ &= \|(A-x)\psi\|^2 + y^2\|\psi\|^2\end{aligned}$$

□

Proof of Theorem 1.3.1. (i) $\Longrightarrow$ (ii): If $A^* = A$, then $\bar{A} = A^{**} = A$ so A is closed. If $\phi \in \operatorname{Ker}(A^* \pm i)$, then by (1.3.1), $0 = \|(A \pm i)\phi\| \geq \|\phi\|$, so $\phi = 0$. Thus, $\operatorname{Ker}(A^* \pm i) = \{0\}$.

(ii) $\Longrightarrow$ (iii): By (1.2.12), $\operatorname{Ran}(A \pm i)^\perp = \operatorname{Ker}(A^* \mp i) = \{0\}$, so $\operatorname{Ran}(A \pm i)$ is dense in $\mathcal{H}$. However, note that $\operatorname{Ran}(A \pm i)$ is closed: if $\phi_n \in \operatorname{Ran}(A \pm i)$ is a Cauchy sequence, $\phi_n = (A \pm i)\psi_n$, then $\|\phi_m - \phi_n\| \geq \|\psi_m - \psi_n\|$ by (1.3.1), so ψ_n is also a Cauchy sequence and closedness of A implies that $(\psi_n, \phi_n \mp i\psi_n)$ has a limit in $\Gamma(A)$. Thus, $\psi_n \to \psi$ and $\phi_n \to \phi = (A \pm i)\psi \in \operatorname{Ran}(A \pm i)$. Since $\operatorname{Ran}(A \pm i)$ is dense and closed, it is equal to $\mathcal{H}$.

(iii) $\Longrightarrow$ (i): We know that $A \subset A^*$, so it suffices to show $D(A^*) \subset D(A)$. Let $\phi \in D(A^*)$. Since $\operatorname{Ran}(A - i) = \mathcal{H}$, there exists $\tilde{\phi} \in D(A)$ such that $(A^* - i)\phi = (A - i)\tilde{\phi}$. Then $(A^* - i)(\phi - \tilde{\phi}) = 0$ by $A \subset A^*$. By $\operatorname{Ran}(A + i) = \mathcal{H}$ and (1.2.12), $\phi - \tilde{\phi} \in \operatorname{Ker}(A^* - i) = \operatorname{Ran}(A + i)^\perp = \{0\}$, so $\phi = \tilde{\phi} \in D(A)$. □

Theorem 1.3.3. *If A is self-adjoint, then $\sigma(A) \subset \mathbb{R}$ and for $z \in \mathbb{C} \setminus \mathbb{R}$,*

$$\|R_z(A)\| \leq \frac{1}{|\operatorname{Im} z|} \tag{1.3.2}$$

Proof. For any $z \in \mathbb{C} \setminus \mathbb{R}$, analogously to the proof of Theorem 1.3.1, it can be shown that $\operatorname{Ker}(A - z) = \{0\}$ and $\operatorname{Ran}(A - z) = \mathcal{H}$. Thus, $A - z$ is a bijection, and its inverse is bounded by $|\operatorname{Im} z|^{-1}$ by (1.3.1), which completes the proof. □

Remark 1.3.1. After proving the spectral theorem, we will be able to improve (1.3.2) to $\|R_z(A)\| = \operatorname{dist}(z, \sigma(A))^{-1}$. However, we will use (1.3.2) to prove the spectral theorem.

For closed, symmetric operators A, one may define

$$K_\pm(A) = \operatorname{Ran}(A \pm i)^\perp = \operatorname{Ker}(A^* \mp i)$$

which are called the *deficiency subspaces* of A. Their dimensions are called the *deficiency indices* of A. They play a crucial role in the description of self-adjoint extensions of A. As we already saw in Theorem 1.3.1, A is self-adjoint if and only if $\dim K_+(A) = \dim K_-(A) = 0$, but more is true: self-adjoint extensions of A are in 1-1 correspondence with unitary maps from $K_+(A)$ to $K_-(A)$ and, in particular, A has self-adjoint extensions if and only if $\dim K_+(A) = \dim K_-(A)$. For details, see [50, Section X.1].

1.4 Essential spectrum and Weyl's theorem

We will now introduce a decomposition of spectrum into two parts and prove a theorem which justifies this decomposition. It is natural to state results in this section for *normal* operators, i.e. operators A such that $AA^* = A^*A$, but all our later applications will be for self-adjoint or unitary operators.

Definition 1.4.1. Let T be a normal operator on $\mathcal{H}$. The *discrete spectrum* of T is

$$\sigma_{\mathrm{d}}(T) = \{\lambda \in \sigma(T) \mid \lambda \text{ is an isolated point of } \sigma(T) \text{ and } \dim \operatorname{Ker}(T-\lambda) < \infty\}$$

and the *essential spectrum* is its complement,

$$\sigma_{\mathrm{ess}}(T) = \sigma(T) \setminus \sigma_{\mathrm{d}}(T)$$

This decomposition is useful because the two types of spectra behave differently under perturbations. For example, for systems such as Jacobi and CMV matrices (described in Chapter 2), it is easy to see that changing a single Jacobi or Verblunsky parameter can change or destroy discrete spectrum. The essential spectrum is much more robust. The concept of essential spectrum was first introduced by Weyl [79], in the context of Schrödinger operators, as that part of the spectrum which doesn't change with varying boundary conditions.

The following is a natural class of perturbations that preserve essential spectrum.

Definition 1.4.2. An operator K is *compact* if it is a norm-limit of finite rank operators, i.e. there exist operators F_n with $\dim \operatorname{Ran} F_n < \infty$ such that

$$\lim_{n\to\infty} \|K - F_n\| = 0$$

Compact operators get their name from a topological property: if $K\colon \mathcal{H} \to \mathcal{H}$ is a compact operator and B a bounded subset of $\mathcal{H}$, then $\overline{K(B)}$ is compact. In fact, this property is often given as the definition of compact operators, but Definition 1.4.2 is more suited to our needs.

We now state without proof a result on the robustness of essential spectrum, due to Weyl [78].

Theorem 1.4.1 (Weyl)**.** *If A and B are normal operators and $A-B$ is compact, then*

$$\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$$

1.5 Examples

In this section, we will give a few examples to illustrate the concepts introduced above.

The first example will be multiplication operators on $L^2(\mathbb{C}, d\mu)$, generalizing and making rigorous a discussion from Section 1.1. Multiplication operators are very simple and many of their properties can be explicitly computed and checked. However, their significance goes beyond that of an example. As we will see in the following sections, the spectral theorem proves that every unitary and self-adjoint operator is unitarily equivalent to a direct sum of multiplication operators!

The remaining few examples in this section will be first-order differential operators. They will illustrate how differential operators can be defined in the framework of unbounded operators on L^2-spaces, and they will illustrate the subtle nature of self-adjointness.

Example 1.5.1. For a positive σ-finite Borel measure μ on $\mathbb{C}$, let $g\colon \mathbb{C} \to \mathbb{C}$ be μ-measurable and let T_g be the operator on $L^2(\mathbb{C}, d\mu)$ defined by

$$D(T_g) = \{f \in L^2(\mathbb{C}, d\mu) \mid g(z)f(z) \in L^2(\mathbb{C}, d\mu)\} \tag{1.5.1}$$

$$(T_g f)(z) = g(z)f(z) \tag{1.5.2}$$

The operator T_g has the following properties:

(i) T_g is densely defined, i.e. $D(T_g)$ is dense in $L^2(\mathbb{C}, d\mu)$.

(ii) T_g is bounded if and only if $g \in L^\infty(\mathbb{C}, d\mu)$; if it is bounded, then $\|T_g\| = \|g\|_\infty$.

(iii) The spectrum of T_g is the essential range of g,

$$\sigma(T_g) = \Big\{\lambda \in \mathbb{C} \mid \mu\big(\{z \mid |g(z) - \lambda| < \epsilon\}\big) > 0 \text{ for all } \epsilon > 0\Big\}$$

and for $\lambda \notin \sigma(T_g)$, the resolvent of T_g at λ is $T_{1/(g-\lambda)}$.

(iv) $T_g^* = T_{\bar{g}}$.

(v) T_g is unitary if and only if $g(z) \in \partial\mathbb{D}$ for μ-a.e. z.

(vi) T_g is self-adjoint if and only if $g(z) \in \mathbb{R}$ for μ-a.e. z.

(vii) If g is bounded on compact sets, then C_0^∞ is a core for T_g.

Proof. (i) Define $A_n = \{z \in \mathbb{C} \mid |g(z)| \le n\}$ for $n \in \mathbb{N}$. For any $f \in L^2(\mathbb{C}, d\mu)$ and any n, $\chi_{A_n} f \in D(T_g)$, but by dominated convergence, $\|f - \chi_{A_n} f\|_2 \to 0$ as $n \to \infty$.

(ii) If $|g(z)| \le M$ for μ-a.e. z, then $\int |g(z)f(z)|^2 d\mu(z) \le M^2 \int |f(z)|^2 d\mu(z)$ so T_g is bounded and $\|T_g\| \le M$. Conversely, assume that $|g(z)| > M$ on a set A with $\mu(A) > 0$. Using σ-finiteness, after possibly restricting to a smaller set A, we can assume $0 < \mu(A) < \infty$. Then with $f(z) = \frac{\chi_A(z)}{\sqrt{\mu(A)}}$, we have $\|f(z)\|_2 = 1$ but $\int |g(z)f(z)|^2 d\mu(z) > M^2$.

(iii) It is easy to see that if $T_g - \lambda$ has a bounded inverse, the inverse is given by the same formal expression as $T_{1/(g-\lambda)}$; by (i), this will be a bounded operator if and only if $\frac{1}{g-\lambda} \in L^\infty(\mathbb{C}, d\mu)$, i.e. if and only if λ is not in the essential range of g.

(iv) For $h \in L^2(\mathbb{C}, d\mu)$, h is in the domain of T_g^* if the map $f \mapsto \int \bar{h} g f \, d\mu$ is a bounded map from $D(T_g)$ to $\mathbb{C}$. If $\bar{h} g \in L^2(\mathbb{C}, d\mu)$, this is true by the Cauchy–Schwarz inequality, and $T_g^* h = \bar{g} h$.

Conversely, if $h \in D(T_g^*)$, then $\int (\bar{h} g - T_g^* h) f \, d\mu = 0$ for all $f \in D(T_g)$. With A_n as in (i), note that $\bar{h} g \chi_{A_n} \in L^2(\mathbb{C}, d\mu)$, so density of $f \chi_{A_n}$ in $L^2(\mathbb{C}, \chi_{A_n} d\mu)$ implies $\bar{h} g \chi_{A_n} = T_{\bar{g}} h \chi_{A_n}$ for all n. Since $\cup_n A_n = \mathbb{C}$, this implies $\bar{h} g = T_{\bar{g}} \in L^2(\mathbb{C}, d\mu)$.

(v) and (vi) follow directly from (iv).

(vii) If g is bounded on compact sets, then $C_0^\infty \subset D(T_g)$. To show that C_0^∞ is a core, first note that by a standard approximation argument, C_0^∞ functions approximate all functions of bounded support in $L^2(\mathbb{C}, d\mu)$, and since g is bounded on compacts, they also approximate them in $L^2(\mathbb{C}, |g|^2 d\mu)$. Finally, if $f \in D(T_g)$, then by a double application of the dominated convergence theorem,

$$\lim_{n \to \infty} \|f - f \chi_{|z| \le n}\|_2^2 = \lim_{n \to \infty} \|gf - gf \chi_{|z| \le n}\|_2^2 = 0$$

so $(f \chi_{|z| \le n}, gf \chi_{|z| \le n})$ approximate (f, gf) in $\mathcal{H} \times \mathcal{H}$, which completes the proof. □

Now we turn to differential operators.

Example 1.5.2. Let $A = -i d/dx$ be an unbounded operator on $L^2(\mathbb{R}, dx)$ with the domain

$$D(A) = \{f \in L^2(\mathbb{R}, dx) \mid f \in \mathrm{AC}_{\mathrm{loc}}(\mathbb{R}), f' \in L^2(\mathbb{R}, dx)\}$$

where $\mathrm{AC}_{\mathrm{loc}}(\mathbb{R})$ is the set of functions absolutely continuous on each compact interval. The operator A is self-adjoint and is unitarily equivalent, via the Fourier transform, to the operator T_x of multiplication by x on $L^2(\mathbb{R}, dx)$. The spectrum of A is $\sigma(A) = \mathbb{R}$.

Proof. To find the adjoint of A, assume that for some $g, h \in L^2(\mathbb{R}, dx)$,

$$\langle g, Af \rangle = \langle h, f \rangle, \quad \forall f \in D(A)$$

Fix a bounded interval $[a, b]$. For $f \in C_0^\infty$ with $\operatorname{supp} f \subset [a, b]$, integration by parts is justified by

$h \in L^2 \subset L^1_{\text{loc}}$ so

$$-\int_a^b \overline{g(x)} i f'(x) dx = \int_a^b \overline{H(x)} f'(x) dx \tag{1.5.3}$$

with $H(x) = \int_a^x h(t)dt$. Note that $h \in L^1_{\text{loc}}$ implies $H \in \text{AC}_{\text{loc}}$.

Pick $j \in C^\infty$ such that $j(x) = 0$ for $x \leq a$ and $j(x) = 1$ for $x \geq b$. Pick $\tilde{f} \in C_0^\infty$ with $\operatorname{supp} \tilde{f} \subset [a, b]$ and let

$$f(x) = \int_a^x \tilde{f}(t)dt - \int_a^b \tilde{f}(t)dt \int_a^x j(t)dt$$

Since $f \in C_0^\infty([a, b])$, plugging this into (1.5.3) and denoting $u(x) = i\overline{g(x)} + \overline{H(x)}$ gives

$$\int_a^b \big[u(x) - \int_a^b u(t)j(t)dt\big] \tilde{f}(x)dx = 0$$

For this to hold for all $\tilde{f} \in C_0^\infty([a, b])$, we must have $u(x) = \int_a^b u(t)j(t)dt$ for a.e. x. By a double application of the Lebesgue differentiation theorem, $H'(x)$ and $u'(x)$ exist for a.e. x and $H'(x) = h(x)$, $u'(x) = 0$, so $ig'(x) = h(x)$ for a.e. x, which shows that $g \in D(A)$ and $h = Ag$. We have thus shown $A^* \subset A$.

For the opposite inclusion, let $f, g \in D(A)$. We will first prove that f, g decay to 0 at $\pm\infty$. Since $f, f' \in L^2$, dominated convergence implies existence of the limit

$$\lim_{R \to +\infty} f(R)^2 - f(0)^2 = \lim_{R \to +\infty} \int_0^R 2f'(x)f(x)dx = \int_0^\infty 2f'(x)f(x)dx$$

and then $f \in L^2$ implies that $\lim_{R \to +\infty} f(R)^2 = 0$ is the only possible value of the limit. By analogy, $\lim_{R \to \pm\infty} f(x)dx = 0$ and $\lim_{R \to \pm\infty} g(x)dx = 0$.

Next, since $\overline{g(x)}f(x) \in \text{AC}_{\text{loc}}$ and $\frac{d}{dx}(\overline{g(x)}f(x)) = \overline{g'(x)}f(x) + \overline{g(x)}f'(x) \in L^1(\mathbb{R}, dx)$, dominated convergence implies

$$\begin{aligned}
\int_{-\infty}^\infty (\overline{g'(x)}f(x) + \overline{g(x)}f'(x))dx &= \lim_{R \to \infty} \int_{-R}^R \frac{d}{dx}(\overline{g(x)}f(x))dx \\
&= \lim_{R \to \infty} (\overline{g(R)}f(R) - \overline{g(-R)}f(-R)) \\
&= 0
\end{aligned}$$

which is equivalent to $\langle Ag, f \rangle = \langle g, Af \rangle$, so $A \subset A^*$. We have thus shown that A is self-adjoint.

For the second part of this example, we remind the reader that the Fourier transform, given by

$$\mathcal{F}(f)(k) = \tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int e^{-ikx} f(x)dx$$

for $f \in \mathcal{S}$ (Schwartz functions), can be extended to an isomorphism of $L^2(\mathbb{R})$. We refer the reader to [50] for details. For $f \in \mathcal{S}$, $k\mathcal{F}(f)(k) = \mathcal{F}(Af)(k)$. Thus, if we define $B = \mathcal{F}A\mathcal{F}^{-1}$ with the domain

$D(B) = \mathcal{F}(D(A))$, then B and T_k are both self-adjoint and agree on $\mathcal{S}$.

Since $C_0^\infty \subset \mathcal{S}$ is a core for T_k, we conclude $T_k = B$, i.e. $T_k = \mathcal{F}A\mathcal{F}^{-1}$. Using this unitary equivalence and the previous example, we see $\sigma(A) = \sigma(T_k) = \mathbb{R}$. □

Our next example is similar, but takes place on a half-line $(0,\infty)$ rather than on $\mathbb{R}$. Note that if $f \in \mathrm{AC}_{\mathrm{loc}}(0,1)$ and $f' \in L^2(0,1)$, then $\int_0^1 |f'(x)|dx \le (\int_0^1 |f'(x)|^2 dx)^{1/2} < \infty$ implies that $f \in \mathrm{AC}[0,1]$, so there is no additional restriction in assuming that functions are absolutely continuous up to the boundary.

Example 1.5.3. Let $A = -id/dx$ be an unbounded operator on $L^2([0,\infty),dx)$ with the domain

$$D(A) = \{f \in L^2([0,\infty),dx) \mid f \in \mathrm{AC}_{\mathrm{loc}}[0,\infty), f' \in L^2([0,\infty),dx)\}$$

The operator A is closed. Its adjoint A^* is a restriction of A to the domain

$$D(A^*) = \{f \in D(A) \mid f(0) = 0\} \tag{1.5.4}$$

The operator A^* is closed and symmetric, but has no self-adjoint extensions. The spectrum of A is $\sigma(A) = \{z \in \mathbb{C} \mid \operatorname{Im} z \ge 0\}$.

Proof. A lot of the considerations from the previous example carry over. The proof that $A^* \subset A$ carries over with no change, but for $f, g \in D(A)$, $\langle Ag, f\rangle = \langle g, Af\rangle$ is equivalent to

$$\begin{aligned}\int_0^\infty (\overline{g'(x)}f(x) + \overline{g(x)}f'(x))dx &= \lim_{R\to\infty} \int_{1/R}^R \frac{d}{dx}(\overline{g(x)}f(x))dx \\ &= \lim_{R\to\infty} (\overline{g(R)}f(R) - \overline{g(1/R)}f(1/R)) \\ &= -\overline{g(0)}f(0)\end{aligned}$$

(since we still know that f and g decay at $+\infty$, by the same argument as in Example 1.5.2). This will be 0 for all $f \in D(A)$ if and only if $g(0) = 0$, which proves (1.5.4). Similarly, one proves $A^{**} = A$, so A is closed.

If B was a self-adjoint extension of A^*, we would have $A^* \subset B \subset A$, but by $\dim(D(A)/D(A^*)) = 1$, this implies $B = A$ or $B = A^*$, neither of which is self-adjoint.

For $\operatorname{Im} z > 0$, $-if'(x) = zf(x)$ has a solution $f(x) = e^{izx} \in D(A)$, so z is an eigenvalue of A. Since the spectrum is a closed set, this implies that $\{z \in \mathbb{C} \mid \operatorname{Im} z \ge 0\} \subset \sigma(A)$. Conversely, for $\operatorname{Im} z < 0$, solving the differential equation $-if' - zf = g$, we claim that the resolvent of A at z is given by

$$(R_z(A)g)(x) = -i\int_x^\infty g(t)e^{iz(x-t)}dt \tag{1.5.5}$$

The integral in (1.5.5) is finite for $g \in L^2(0,\infty)$ because $e^{iz(x-t)}$ decays exponentially at infinity, and denoting $f = R_z(A)g$ and $k = -\operatorname{Im} z$,

$$|f(x)| \leq \int_x^\infty |g(t)| e^{-k(t-x)} dt$$

so by an application of Tonelli's theorem,

$$\begin{aligned}
\int_0^\infty |f(x)|^2 dx &\leq \int_0^\infty \int_x^\infty \int_x^\infty |g(s)| e^{-k(s-x)} |g(t)| e^{-k(t-x)} ds\, dt\, dx \\
&= \int_0^\infty \int_0^\infty \int_0^{\min(s,t)} |g(s)||g(t)| e^{-k(s+t-2x)} dx\, ds\, dt \\
&\leq \frac{1}{2k} \int_0^\infty \int_0^\infty |g(s)||g(t)| e^{-k|s-t|} ds\, dt
\end{aligned}$$

We will now introduce the change of variables $s = u + v$, $t = u - v$; in order not to worry about limits of integration, it will be convenient to think of g as an element of $L^2(\mathbb{R}, dx)$ with $g(x) = 0$ for $x < 0$. Using the Cauchy–Schwarz inequality,

$$\begin{aligned}
\int_0^\infty |f(x)|^2 dx &\leq \frac{1}{k} \int_{-\infty}^\infty \int_{-\infty}^\infty |g(u+v)||g(u-v)| e^{-2k|v|} du\, dv \\
&\leq \frac{1}{k} \int_{-\infty}^\infty \|g\|_2^2 e^{-2k|v|} dv \\
&\leq \frac{1}{k^2} \|g\|_2^2
\end{aligned}$$

which shows that $R_z(A)$ is a bounded operator on $\mathcal{H}$. That $f \in \mathrm{AC}_{\mathrm{loc}}[0,\infty)$ and $-if' - zf = g$ follows from the integral equality

$$f(x) = f(0) + \int_0^x [zf(s) + g(s)] ds$$

which is easy to verify by using the definition of f and Fubini's theorem. Thus, $R_z(A)$ is indeed a bounded two-sided inverse for $A - z$, so $z \notin \sigma(A)$ for $\operatorname{Im} z < 0$. □

Whereas in the previous example, an operator had no self-adjoint extensions, the next example will be of an operator with infinitely many self-adjoint extensions. Moreover, we will see that the choice of self-adjoint extension affects the spectrum.

Example 1.5.4. Let $A = -id/dx$ be an unbounded operator on $L^2([0,1], dx)$ with the domain

$$D(A) = \{f \in L^2([0,1], dx) \mid f \in \mathrm{AC}[0,1], f' \in L^2([0,1], dx)\}$$

The operator A is closed. Its adjoint A^* is a restriction of A to the domain

$$D(A^*) = \{f \in D(A) \mid f(0) = f(1) = 0\} \tag{1.5.6}$$

The operator A^* is closed and symmetric. Its self-adjoint extensions A_ω are parametrized by $\omega \in \partial\mathbb{D}$ and given by

$$D(A_\omega) = \{f \in D(A) \mid f(1) = \omega f(0)\} \tag{1.5.7}$$

For $\omega = e^{ik}$, the spectrum of A_ω is $\sigma(A_\omega) = k + 2\pi\mathbb{Z}$.

Proof. Performing an analysis analogous to the previous two examples, we see that $A^* \subset A$ and for $f, g \in D(A)$,

$$\langle f, Ag\rangle - \langle Af, g\rangle = -i(\overline{f(1)}g(1) - \overline{f(0)}g(0)) \tag{1.5.8}$$

which implies (1.5.6). If $A^* \subsetneq B \subsetneq A$, then $D(B) = D(A^*) \oplus \mathbb{C}h$ for some $h \in D(A)$, which is of the form (1.5.7) with $\omega = h(1)/h(0)$ (we allow $\omega \in \mathbb{C} \cup \{\infty\}$), so $B = A_\omega$ for some $\omega \in \mathbb{C} \cup \{\infty\}$. Using (1.5.8), we see that $A_\omega^* = A_{1/\bar\omega}$, so A_ω is self-adjoint if and only if $\omega \in \partial\mathbb{D}$.

For $\omega = e^{ik}$, note that $e^{i(2\pi n+k)x} \in D(A_\omega)$ for $n \in \mathbb{Z}$ and that $A_\omega e^{i(2\pi n+k)x} = (2\pi n+k)e^{i(2\pi n+k)x}$, so $2\pi n + k$ are eigenvalues of A_ω. For $z \notin k + 2\pi\mathbb{Z}$, finding the solution of $-if' - zf = g$ with $f(1)/f(0) = \omega$, we may conjecture that the resolvent of A_ω at z is given by

$$(R_z(A_\omega)g)(x) = \frac{i}{e^{i(k-z)} - 1}\left[e^{i(k-z)}\int_0^x g(t)e^{iz(x-t)}dt + \int_x^1 g(t)e^{iz(x-t)}dt\right]$$

and similarly to the previous example, it is straightforward to verify that this is, indeed, the resolvent, so $\sigma(A_\omega) = k + 2\pi\mathbb{Z}$. □

All of the differential operators considered here were first-order differential operators. Second-order differential operators will be the subject of Chapter 3.

1.6 A digression: Carathéodory and Herglotz functions

This section is not about linear operators, but it describes background material in complex analysis which will be important throughout this text. We will define two classes of complex analytic functions and establish a 1-1 correspondence between them and finite probability measures on the unit circle and real line via the complex Poisson transform and the Stieltjes transform (to be defined below).

Carathéodory functions were first studied by Carathéodory [10], who was interested in conditions on Taylor coefficients under which an analytic function on $\mathbb{D}$ has positive real part. The correspondence with positive measures on $\partial\mathbb{D}$ is due to Herglotz [29] and Riesz [55]. The analogue on the upper half-plane has been studied most by Herglotz, Nevanlinna and Pick, so what we call Herglotz functions below also appear in the literature as Nevanlinna or Pick functions. The connection of these functions with measures on the real line is due to Borel and Stieltjes.

Definition 1.6.1. A Carathéodory function is an analytic function $F\colon \mathbb{D} \to \{z \in \mathbb{C} \mid \operatorname{Re} z > 0\}$ with $F(0) = 1$. A Herglotz function is an analytic function $f\colon \mathbb{C}_+ \to \mathbb{C}_+$.

Definition 1.6.2. Let μ be a finite positive measure on $\partial\mathbb{D}$. Its *complex Poisson transform* is an analytic function on $\mathbb{D}$, given by

$$F(z) = \int_{\partial\mathbb{D}} \frac{e^{i\theta} + z}{e^{i\theta} - z} d\mu(e^{i\theta}) \tag{1.6.1}$$

For a finite positive measure ρ on $\mathbb{R}$, its *Stieltjes transform* is an analytic function on $\mathbb{C}_+$,

$$f(z) = \int \frac{1}{x - z} d\rho(x) \tag{1.6.2}$$

The following theorem establishes the announced correspondence for measures on the unit circle.

Theorem 1.6.1 (Herglotz representation)**.** *The formula*

$$F(z) = i\beta + \int_{\partial\mathbb{D}} \frac{e^{i\theta} + z}{e^{i\theta} - z} d\mu(e^{i\theta}) \tag{1.6.3}$$

provides a 1-1 correspondence between analytic maps from $\mathbb{D}$ *to* $\{z \in \mathbb{C} \mid \operatorname{Re} z > 0\}$ *and pairs* (β, μ) *with* $\beta \in \mathbb{R}$ *and* μ *a positive finite measure on* $\partial\mathbb{D}$*. The inverse map is given by* $\beta = \operatorname{Im} F(0)$ *and*

$$d\mu(\theta) = \operatorname*{w-lim}_{r\uparrow 1} \operatorname{Re} F(re^{i\theta}) \frac{d\theta}{2\pi}$$

In particular, the formula (1.6.1) *provides a 1-1 correspondence between probability measures on* $\partial\mathbb{D}$ *and Carathéodory functions.*

For the proof, we will need the complex Poisson representation: for f analytic in a neighborhood of $\overline{\mathbb{D}}$ and $z \in \mathbb{D}$,

$$f(z) = i \operatorname{Im} f(0) + \int \frac{e^{i\theta} + z}{e^{i\theta} - z} \operatorname{Re} f(e^{i\theta}) \frac{d\theta}{2\pi} \tag{1.6.4}$$

For a proof of (1.6.4), see [57].

Proof of Theorem 1.6.1. Direct calculations show

$$\operatorname{Re} F(z) = \int \frac{1 - |z|^2}{|e^{i\theta} - z|^2} d\mu(e^{i\theta})$$

so (1.6.3) defines a map from $\mathbb{D}$ to $\{z \in \mathbb{C} \mid \operatorname{Re} z > 0\}$ for any finite positive measure μ. Now fix

$F(z)$ and define positive measures μ_r on $\partial\mathbb{D}$ for $r < 1$ by

$$d\mu_r(e^{i\theta}) = \operatorname{Re} F(re^{i\theta})\frac{d\theta}{2\pi}$$

Since $F(z)$ is analytic in $\mathbb{D}$, it has an absolutely convergent power series $F(z) = c_0 + 2\sum_{n=1}^{\infty} c_n z^n$, which implies that $\operatorname{Re} F(re^{i\theta}) = \sum_{n=-\infty}^{\infty} c_{|n|} r^{|n|} e^{in\theta}$. Then moments of μ_r are

$$\int e^{-in\theta} d\mu_r(\theta) = c_{|n|} r^{|n|} \tag{1.6.5}$$

Note that the μ_r are positive measures with $\mu_r(\partial\mathbb{D}) = c_0$, and that (1.6.5) converges as $r \uparrow 1$ for every n, so density of trigonometric polynomials in $C(\partial\mathbb{D})$ shows that $d\mu_r$ have a weak limit, $d\mu$, such that $\int e^{-in\theta} d\mu(\theta) = c_{|n|}$. But the complex Poisson representation implies

$$F(rz) = i\beta + \int \frac{e^{i\theta} + z}{e^{i\theta} - z} d\mu_r(e^{i\theta})$$

with $\beta = \operatorname{Im} F(0)$ so taking the limit $r \uparrow 1$ implies (1.6.3).

In particular, letting $z = 0$ in (1.6.3) gives $F(0) = i\beta + \mu(\partial\mathbb{D})$, so F is Carathéodory if and only if $\beta = 0$ and μ is a probability measure. □

Theorem 1.6.2 (Stieltjes representation)**.** *Let f be a Herglotz function. Then there exists a unique positive measure ρ on $\mathbb{R}$ with $\int \frac{1}{1+x^2} d\rho(x) < \infty$ and constants $\alpha \in \mathbb{R}$, $\gamma \geq 0$ such that*

$$f(z) = \alpha + \gamma z + \int_{\mathbb{R}} \left(\frac{1}{x - z} - \frac{x}{1 + x^2} \right) d\rho(x) \tag{1.6.6}$$

In particular, if and only if $\sup_{y>0}|yf(iy)| < \infty$, f has the representation (1.6.2) *with ρ a finite positive measure on $\mathbb{R}$, and in that case $\sup_{y>0}|yf(iy)| = \rho(\mathbb{R})$.*

Proof. We will need the fractional linear transformation $\Gamma(w) = i\frac{1+w}{1-w}$ which maps $\mathbb{D}$ onto $\mathbb{C}_+$. Note that f is Herglotz if and only if $F = -if \circ \Gamma$ is a map from $\mathbb{D}$ to $\{z \mid \operatorname{Re} z > 0\}$. We will thus use Theorem 1.6.1 and perform a conformal change of variables. If μ is a positive bounded measure on $\partial\mathbb{D}$, we can define ρ as

$$d\rho(x) = (1 + x^2) d\mu(\Gamma^{-1}(x))$$

Note that Γ is a bijection between $\partial\mathbb{D}\backslash\{1\}$ and $\mathbb{R}$, so a change of variables shows that, with $z = \Gamma(w)$ and $x = \Gamma(e^{i\theta})$,

$$i\beta + \int_{\partial\mathbb{D}} \frac{e^{i\theta} + w}{e^{i\theta} - w} d\mu(e^{i\theta}) = i\beta - i\mu(\{1\})z + \int_{\mathbb{R}} \left(\frac{1}{x - z} - \frac{x}{1 + x^2} \right) d\rho(x)$$

Also note that $\int_{\mathbb{R}} \frac{1}{1+x^2} d\rho(x) = \mu(\partial\mathbb{D}) - \mu(\{1\})$. Thus, with $\alpha = -\beta$ and $\gamma = \mu(\{1\})$, existence and uniqueness of the representation (1.6.6) follow directly from Theorem 1.6.1.

For the second part of the theorem, note that if (1.6.2) with $\rho(\mathbb{R}) < \infty$, then $|x - iy| \geq y$ implies $|f(iy)| \leq \rho(\mathbb{R})/y$ for all $y > 0$. For the converse, let $M = \sup_{y>0}|yf(iy)| < \infty$. Then $|y \operatorname{Re} f(iy)|, |y \operatorname{Im} f(iy)| \leq M$, so using (1.6.6), we get

$$|y \operatorname{Re} f(iy)| = \left| \alpha y + \int_{\mathbb{R}} \left(\frac{xy}{x^2+y^2} - \frac{xy}{1+x^2} \right) d\rho(x) \right| \leq M \tag{1.6.7}$$

$$|y \operatorname{Im} f(iy)| = \left| \gamma y^2 + \int_{\mathbb{R}} \frac{y^2}{x^2+y^2} d\rho(x) \right| \leq M \tag{1.6.8}$$

Since both γy^2 and $\int_{\mathbb{R}} \frac{y^2}{x^2+y^2} d\rho(x)$ are positive, (1.6.8) implies $\gamma y^2 \leq M$ for all $y > 0$, so $\gamma = 0$. (1.6.8) then also implies $\int_{\mathbb{R}} \frac{y^2}{x^2+y^2} d\rho(x) \leq M$. From this estimate and the monotone convergence theorem,

$$\rho(\mathbb{R}) = \int_{\mathbb{R}} \lim_{y\to\infty} \frac{y^2}{x^2+y^2} d\rho(x) = \lim_{y\to\infty} \int_{\mathbb{R}} \frac{y^2}{x^2+y^2} d\rho(x) \leq M$$

Meanwhile, dividing (1.6.7) by y and taking the limit as $y \to \infty$, we have

$$\alpha = \lim_{y\to\infty} \int_{\mathbb{R}} \left(\frac{x}{1+x^2} - \frac{x}{x^2+y^2} \right) d\rho(x) = \int_{\mathbb{R}} \frac{x}{1+x^2} d\rho(x)$$

since for $y \geq 1$ the integrand is non-negative and increasing in y, so the monotone convergence theorem applies. Combining these conclusions into (1.6.6) gives precisely (1.6.2). $\square$

As the final result in this section, we present a corollary which we will need in Section 1.8.

Corollary 1.6.3. *If $d\nu$ is a finite complex measure such that*

$$\int_{\mathbb{R}} \frac{1}{x-z} d\nu(x) = 0, \quad \forall z \in \mathbb{C} \setminus \mathbb{R} \tag{1.6.9}$$

then $\nu = 0$.

Proof. We will use the notation $f[\nu](z) = \int_{\mathbb{R}} \frac{1}{x-z} d\nu$ for any finite measure ν. Let us first prove the claim for real (signed) measures. Using the decomposition $\nu = \nu_+ - \nu_-$ into a difference of two positive measures, we see $f[\nu] = 0$ implies $f[\nu_+] = f[\nu_-]$, so by uniqueness of the Stieltjes transform, $\nu_+ = \nu_-$ and $\nu = 0$.

If ν is a complex measure, using $\overline{f[\nu](z)} = f[\overline{\nu}](\bar{z})$ and combining with the original equation, we see that $f[\operatorname{Re} \nu](z) = f[\operatorname{Im} \nu](z) = 0$, so by the previous part, $\operatorname{Re} \nu = \operatorname{Im} \nu = 0$. $\square$

1.7 Spectral theorem for unitary operators

We now move on to the spectral theorem. We are interested in two classes of operators: unitary and self-adjoint operators. Since unitary operators are bounded and so technically easier to handle, we discuss the unitary case first and discuss the self-adjoint case in the next section.

Theorem 1.7.1 (Spectral theorem for unitary operators)**.** *Let U be a unitary operator on $\mathcal{H}$. There exists a sequence of probability measures $(d\mu_n)_{n=1}^N$ on $\partial\mathbb{D}$ (N may be finite or infinite) and a unitary map*

$$W\colon \bigoplus_{n=1}^{N} L^2(\partial\mathbb{D}, d\mu_n) \to \mathcal{H} \tag{1.7.1}$$

such that for every $f = (f_n)_{n=1}^N \in \bigoplus_{n=1}^N L^2(\partial\mathbb{D}, d\mu_n)$,

$$(W^{-1}UWf)_n(e^{i\theta}) = e^{i\theta} f_n(e^{i\theta}) \tag{1.7.2}$$

A representation with $N = 1$ exists if and only if U has a cyclic vector.

We remind the reader that a direct sum of Hilbert spaces, $\mathcal{H} = \bigoplus_{n=1}^N \mathcal{H}_n$, is the Hilbert space of sequences $(f_n)_{n=1}^N$ such that $f_n \in \mathcal{H}_n$, $\sum_{n=1}^N \|f_n\|^2 < \infty$ with the inner product

$$\langle f, g\rangle_{\mathcal{H}} = \sum_{n=1}^{N} \langle f_n, g_n\rangle_{\mathcal{H}_n}$$

The bulk of the proof concerns the special case for which one can take $N = 1$. The appropriate condition for this to be possible is given by the following definition.

Definition 1.7.1. Let U be a unitary operator on $\mathcal{H}$. The *cyclic subspace generated by* $\psi \in \mathcal{H}$ is $C_U(\psi) = \operatorname{span}\{U^n\psi \mid n \in \mathbb{Z}\}$. The vector ψ is a *cyclic vector* for U if $\overline{C_U(\psi)} = \mathcal{H}$. If U has a cyclic vector, it is said to have *simple spectrum.*

Remark 1.7.1. If $\mathcal{H}$ is finite-dimensional, U has a cyclic vector if and only if it has no repeated eigenvalues.

Theorem 1.7.2 (Spectral theorem for unitary operators with a cyclic vector)**.** *Let $U\colon \mathcal{H} \to \mathcal{H}$ be unitary and let $\psi \in \mathcal{H}$. Then there exists a unique positive Borel measure $\mu_\psi(\theta)$ on $[0, 2\pi)$ such that for all $n \in \mathbb{Z}$,*

$$\langle \psi, U^n\psi\rangle = \int_0^{2\pi} e^{in\theta} d\mu_\psi(\theta) \tag{1.7.3}$$

The measure satisfies $\mu_\psi(\partial\mathbb{D}) = \|\psi\|_2^2$. Moreover, there exists a unitary operator $W\colon L^2(\partial\mathbb{D}, d\mu_\psi) \to \overline{C_U(\psi)}$ such that

$$(W^{-1}UWf)(e^{i\theta}) = e^{i\theta} f(e^{i\theta}) \tag{1.7.4}$$

for all $f \in L^2(\partial\mathbb{D}, d\mu_\psi)$.

For the proof we will need a theorem of Fejér [17] and Riesz [56].

Lemma 1.7.3 (Fejér–Riesz Theorem). *If f is a Laurent polynomial, i.e. $f(z) = \sum_{n=M}^{N} a_n z^n$ with $M, N \in \mathbb{Z}$, and if $f(z) \geq 0$ for all $z \in \partial\mathbb{D}$, then there exists a polynomial P whose zeros are all in $\bar{\mathbb{D}}$, such that*

$$f(z) = P(z)\overline{P(1/\bar{z})} \tag{1.7.5}$$

Proof. Since $f(z)$ and $\overline{f(1/\bar{z})}$ are analytic functions of z which coincide on $\partial\mathbb{D}$, they must be equal, i.e.

$$f(z) = \overline{f(1/\bar{z})} \tag{1.7.6}$$

Writing f in the form $f(z) = z^M Q(z)$ with Q a polynomial, we see that f can be decomposed as a product of linear factors,

$$f(z) = Az^M \prod_{k=1}^{K} (z - z_k)^{j_k} \tag{1.7.7}$$

where the z_k are distinct and j_k are their multiplicities. Substituting this on both sides of (1.7.6), we see that for every zero z_k of f, $1/\bar{z}_k$ is a zero of the same multiplicity. Since $f(z)$ has constant sign on $\partial\mathbb{D}$, zeros on $\partial\mathbb{D}$ have even multiplicity. Thus, one can take P to be a constant B times the product of $(z - z_k)^{i_k}$ where

$$i_k = \begin{cases} j_k, & |z_k| < 1 \\ j_k/2, & |z_k| = 1 \\ 0, & |z_k| > 1 \end{cases}$$

For a suitable choice of B, we get a polynomial such that (1.7.5) holds. □

Proof of Theorem 1.7.2. We begin by constructing a linear functional Λ on the space T of Laurent polynomials. Define Λ by

$$\Lambda\Big(\sum_{j=k}^{l} c_j e^{ij\theta}\Big) = \Big\langle \psi, \sum_{j=k}^{l} c_j U^j \psi \Big\rangle$$

If $\sum_{j=k}^{l} c_j e^{ij\theta} \geq 0$ for all $\theta \in \mathbb{R}$, then by Lemma 1.7.3, $\sum_{j=k}^{l} c_j z^j = P(z)\overline{P(1/\bar{z})}$. Since $U^* = U^{-1}$, this implies $\sum_{j=k}^{l} c_j U^j = P(U)P(U)^*$ and

$$\Lambda\Big(\sum_{j=k}^{l} c_j e^{ij\theta}\Big) = \langle \psi, P(U)^* P(U)\psi \rangle = \langle P(U)\psi, P(U)\psi \rangle \geq 0$$

Thus, Λ is a positive functional on T.

If $\|\sum_{j=k}^{l} c_j e^{ij\theta}\|_\infty \leq 1$, then $1 \pm \operatorname{Re} \sum_{j=k}^{l} c_j e^{ij\theta} \geq 0$ and $1 \pm \operatorname{Im} \sum_{j=k}^{l} c_j e^{ij\theta} \geq 0$ for all θ. Since the real and imaginary parts of trigonometric polynomials are trigonometric polynomials and by positivity of Λ,

$$\pm\Lambda\Big(\mathrm{Re}\sum_{j=k}^{l} c_j e^{ij\theta}\Big) \le \Lambda(1) = \|\psi\|_2^2$$
$$\pm\Lambda\Big(\mathrm{Im}\sum_{j=k}^{l} c_j e^{ij\theta}\Big) \le \Lambda(1) = \|\psi\|_2^2$$

From this we see $\big|\Lambda\big(\sum_{j=k}^{l} c_j e^{ij\theta}\big)\big| \le 2\|\psi\|_2^2$, so Λ is a bounded functional on T if T is equipped with the L^∞-norm.

By the Weierstrass approximation theorem, T is a dense subspace of $C(\partial\mathbb{D})$, so Λ extends to a bounded, positive functional on $C(\partial\mathbb{D})$. Thus, by the Riesz–Markov theorem, there exists a unique positive measure μ_ψ such that $\Lambda(f) = \int f(\theta) d\mu_\psi(\theta)$.

Next, $|\Lambda(f)| \le \int |f(\theta)| d\mu_\psi(\theta) \le \|f\|_\infty \mu_\psi(\partial\mathbb{D})$ with equality for $f(\theta) \equiv 1$ implies that $\|\Lambda\| = \mu_\psi(\partial\mathbb{D}) = \Lambda(1) = \|\psi\|_2^2$.

We proceed to construct W. First define W on T by

$$W\big(\sum_{j=k}^{l} c_j e^{ij\theta}\big) = \sum_{j=k}^{l} c_j U^j \psi$$

Viewing T as a subspace of $L^2(\mathbb{D}, d\mu)$, W is a norm-preserving map from T to $C_U(\psi)$ because

$$\begin{aligned}
\Big\| W\Big(\sum_{j=k}^{l} c_j e^{ij\theta}\Big)\Big\|^2 &= \Big\langle \sum_{j=k}^{l} c_j U^j \psi, \sum_{j=k}^{l} c_j U^j \psi \Big\rangle \\
&= \Big\langle \psi, \sum_{j=k}^{l} \bar{c}_j U^{-j} \sum_{j=k}^{l} c_j U^j \psi \Big\rangle \\
&= \Lambda\Big(\sum_{j=k}^{l} \bar{c}_j e^{-ij\theta} \sum_{j=k}^{l} c_j e^{ij\theta}\Big) \\
&= \int \Big|\sum_{j=k}^{l} c_j e^{ij\theta}\Big|^2 d\mu_\psi(\theta)
\end{aligned}$$

Since T is dense in $L^2(\partial\mathbb{D}, d\mu)$, this means that W can be uniquely extended to a unitary map of $L^2(\mathbb{D}, d\mu)$ onto $\overline{C_U(\psi)}$. Finally, it is straightforward to check that (1.7.4) is satisfied for $f \in T$, and since $W^{-1}UW$ and multiplication by $e^{i\theta}$ are both unitary operators on $L^2(\mathbb{D}, d\mu)$, agreement on a dense set is sufficient to conclude that they are equal. □

Proof of Theorem 1.7.1. We start by proving that $\mathcal{H}$ can be written as an at most countable direct sum of closures of cyclic subspaces. Since $\mathcal{H}$ is separable, it has an (at most countable) orthonormal basis $\{\phi_n\}_{n=1}^N$. We define $\{\psi_n\}_{n=1}^N$ inductively: let $\psi_1 = \phi_1$ and let ψ_n be the orthogonal projection of ϕ_n onto $V_{n-1} = \cap_{k=1}^{n-1}(C_U(\psi_k)^\perp)$.

Since $\psi_n \perp C_U(\psi_k)$ for $k < n$ and U is unitary, we have $U^i\psi_n \perp U^j\psi_k$ for $i, j \in \mathbb{Z}$ so

$$\overline{C_U(\psi_n)} \cap \overline{C_U(\psi_k)} = \{0\} \text{ for } n \neq k \tag{1.7.8}$$

Thus, sums of the $\overline{C_U(\psi_n)}$ are direct sums and $V_{n-1} = (\bigoplus_{k=1}^{n-1} \overline{C_U(\psi_k)})^\perp$. It follows from the construction that $\phi_n \in \bigoplus_{k=1}^{n} \overline{C_U(\psi_k)}$, so since $\{\phi_n\}_{n=1}^N$ is an ONB of $\mathcal{H}$,

$$\mathcal{H} = \bigoplus_{n=1}^{N} \overline{C_U(\psi_n)} \tag{1.7.9}$$

Note that this construction served only to provide existence of ψ_n with the property (1.7.9). We may try to impose additional restrictions on $\{\psi_n\}$, as long as we preserve the property (1.7.9). For example, we may discard from the sequence all ψ_n which are equal to 0 and normalize all the others to get the condition $\|\psi_n\| = 1$ for all n as stated in the theorem.

By Theorem 1.7.2, there exist measures μ_n and unitaries $W_n : L^2(\partial\mathbb{D}, d\mu_n) \to \overline{C_U(\psi_n)}$ such that $(W_n^{-1} U W_n f_n)(e^{i\theta}) = e^{i\theta} f_n(e^{i\theta})$ for $f_n \in L^2(\partial\mathbb{D}, d\mu_n)$. Taking $W = \bigoplus_{n=1}^N W_n$, we get a unitary operator $W : \bigoplus_{n=1}^N L^2(\partial\mathbb{D}, d\mu_n) \to \mathcal{H}$ satisfying (1.7.2).

If U has a cyclic vector, we could have picked ψ_1 to be the cyclic vector and $N = 1$. Conversely, if U has a spectral representation with $N = 1$, then taking $\psi = W(1)$, we have $U^n\psi = W(e^{in\theta})$ so density of T in $L^2(\partial\mathbb{D}, d\mu_1)$ implies density of $C_U(\psi)$ in $\mathcal{H}$ and ψ is a cyclic vector. □

In Section 1.9, we will discuss some corollaries of the spectral theorem.

1.8 Spectral theorem for self-adjoint operators

In this section, we state and prove the spectral theorem for self-adjoint operators.

Definition 1.8.1. For an unbounded self-adjoint operator A and $\psi \in \mathcal{H}$, we define the cyclic subspace of ψ as

$$C_A(\psi) = \operatorname{span}\{(A - z)^{-1}\psi \mid z \in \mathbb{C} \setminus \mathbb{R}\}$$

A vector ψ is cyclic if and only if $\overline{C_A(\psi)} = \mathcal{H}$.

This definition is different than the one given for unitary operators. Indeed, here it would not be suitable to define the cyclic subspace as the span of $A^n\psi$, because ψ might not be in the domains of the A^n. However, in Corollary 1.9.2 we will show that for a bounded self-adjoint operator, the other definition would produce a set with the same closure.

Theorem 1.8.1 (Spectral theorem for self-adjont operators). *Let A be a self-adjoint operator on $\mathcal{H}$. There exists a sequence of probability measures $\{d\mu_n\}_{n=1}^N$ (with N finite or infinite) and a unitary* *map*

$$W\colon \bigoplus_{n=1}^{N} L^2(\mathbb{R}, d\mu_n) \to \mathcal{H} \tag{1.8.1}$$

such that

$$D(A) = W\left(\left\{f \in \bigoplus_{n=1}^{N} L^2(\mathbb{R}, d\mu_n) \,\middle|\, \sum_{n=1}^{N} \int |xf_n(x)|^2 d\mu_n(x) < \infty\right\}\right)$$

and for every $f \in \bigoplus_{n=1}^{N} L^2(\mathbb{R}, d\mu_n)$,

$$(W^{-1}AWf)_n(x) = xf_n(x) \tag{1.8.2}$$

A representation with $N = 1$ *exists if and only if* A *has a cyclic vector.*

Theorem 1.8.2 (Spectral theorem for self-adjoint operators with a cyclic vector)**.** *Let* A *be a densely defined self-adjoint operator and* $\psi \in \mathcal{H}$*. There exists a unique positive Borel measure* μ_ψ *on* $\mathbb{R}$ *such that for all* $z \in \mathbb{C}_+$,

$$\langle \psi, (A-z)^{-1}\psi\rangle = \int \frac{1}{x-z} d\mu_\psi(x) \tag{1.8.3}$$

Moreover, μ_ψ *is a finite measure with* $\mu_\psi(\mathbb{R}) = \|\psi\|^2$*. There exists a unitary map* $W\colon L^2(\mathbb{R}, d\mu_\psi) \to \overline{C_A(\psi)}$ *such that* $W1 = \psi$,

$$D(A) = W\left(\left\{f \in L^2(\mathbb{R}, d\mu_\psi) \middle| \int |xf(x)|^2 d\mu_\psi(x) < \infty\right\}\right) \tag{1.8.4}$$

and

$$(W^{-1}AWf)(x) = xf(x) \tag{1.8.5}$$

Proof. Let us define $B(z) = \langle \psi, (A-z)^{-1}\psi\rangle$ for $\operatorname{Im} z > 0$. We will prove that $B(z)$ is a Herglotz function. Since $A = A^*$, $R_z(A)^* = R_{\bar{z}}(A)$ so using (1.2.3),

$$\begin{aligned}
\operatorname{Im} B(z) &= \frac{1}{2i}(\langle \psi, R_z(A)\psi\rangle - \langle R_z(A)\psi, \psi\rangle) \\
&= \frac{1}{2i}\langle \psi, R_z(A) - R_{\bar{z}}(A)\psi\rangle \\
&= \frac{1}{2i}(z-\bar{z})\langle \psi, R_{\bar{z}}(A)R_z(A)\psi\rangle \\
&= \operatorname{Im} z \, \|R_z(A)\psi\|^2
\end{aligned}$$

By Theorem 1.2.1, $R_z(A)$ is norm-analytic in $z \in \mathbb{C}_+$, so $B(z)$ is analytic in $z \in \mathbb{C}_+$. Thus, $B(z)$ is a Herglotz function. By (1.3.2), $|B(iy)| \le \|R_{iy}(A)\|\|\psi\|^2 \le \frac{1}{y}\|\psi\|^2$, so existence and uniqueness of μ_ψ follows from Theorem 1.6.2, as well as the bound $|\mu_\psi(\mathbb{R})| \le \|\psi\|^2$.

Taking the complex conjugate of (1.8.3) and using $R_z(A)^* = R_{\bar{z}}(A)$, we conclude that (1.8.3) also holds when $\operatorname{Im} z < 0$. Thus, using (1.2.3), for $z, w \in \mathbb{C} \setminus \mathbb{R}$, $z \neq \bar{w}$ we have

$$\begin{aligned}\langle R_w(A)\psi, R_z(A)\psi\rangle &= \langle \psi, R_{\bar{w}}(A)R_z(A)\psi\rangle \\ &= \frac{1}{z-\bar{w}}(\langle \psi, R_z(A)\psi\rangle - \langle \psi, R_{\bar{w}}(A)\psi\rangle) \\ &= \frac{1}{z-\bar{w}}\left(\int \frac{1}{x-z} d\mu_\psi(x) - \int \frac{1}{x-\bar{w}} d\mu_\psi(x)\right) \\ &= \int \overline{\left(\frac{1}{x-w}\right)} \frac{1}{x-z} d\mu_\psi(x)\end{aligned}$$

However, note that both sides of

$$\langle R_w(A)\psi, R_z(A)\psi\rangle = \int \overline{\left(\frac{1}{x-w}\right)} \frac{1}{x-z} d\mu_\psi(x) \tag{1.8.6}$$

are continuous in z away from $\mathbb{R}$, by norm-continuity of $R_z(A)$ and continuity of the integral in z (by a simple dominated convergence argument, since the integrand is uniformly bounded and μ_ψ is a finite measure). Thus, taking the limit of this equality as $z \to \bar{w}$, we conclude that (1.8.6) holds for $z = \bar{w}$ as well. Finally, by linearity for any finite sequence $c_1, \dots, c_J \in \mathbb{C}$, $z_1, \dots, z_J \in \mathbb{C} \setminus \mathbb{R}$,

$$\left\| \sum_{j=1}^{J} c_j R_{z_j}(A)\psi \right\|^2 = \int \left| \sum_{j=1}^{J} c_j \frac{1}{x-z_j} \right|^2 d\mu_\psi(x) \tag{1.8.7}$$

Define $V = \operatorname{span}\{\frac{1}{x-z} \mid z \in \mathbb{C} \setminus \mathbb{R}\} \subset L^2(\mathbb{R}, d\mu)$. We can define a linear map $W \colon V \to \mathcal{H}$ by $W\frac{1}{x-z} = R_z(A)\psi$ and this map is well-defined since, by (1.8.7), $\sum_{j=1}^{J} c_j \frac{1}{x-z_j} = 0$ μ-a.e. implies that $\sum_{j=1}^{J} c_j R_{z_j}(A)\psi = 0$. Moreover, (1.8.7) implies that W is norm-preserving.

If $f \perp V$, then for all $z \in \mathbb{C} \setminus \mathbb{R}$ we have $\int_{\mathbb{R}} \frac{1}{x-z} \overline{f(x)} d\mu_\psi(x) = 0$, so Corollary 1.6.3 implies that $f d\mu_\psi = 0$, so $f = 0$ in $L^2(\mathbb{R}, d\mu_\psi)$. Thus, V is a dense subspace of $L^2(\mathbb{R}, d\mu_\psi)$, so W extends uniquely to a unitary map from $L^2(\mathbb{R}, d\mu_\psi)$ to $\overline{C_A(\psi)}$.

For $f \in L^2(\mathbb{R}, d\mu_\psi)$, Wf is in the domain of A if and only if $Wf = (A-i)^{-1}\phi$ for some $\phi \in \mathcal{H}$. Denoting $g = W^{-1}\phi$, we conclude that $f \in W^{-1}(D(A))$ if and only if $f(x) = \frac{1}{x-i} g(x)$ for some $g \in L^2(\mathbb{R}, d\mu_\psi)$, which is equivalent to $xf(x) \in L^2(\mathbb{R}, d\mu_\psi)$. Finally, $Wf = (A-i)^{-1}Wg$ implies $AWf = iWf + Wg = W(if + (x-i)f) = W(xf)$, so (1.8.5) holds. □

Proof of Theorem 1.8.1. Given Theorem 1.8.2, the proof is entirely analogous to the proof of Theorem 1.7.1. □

1.9 Applications of the spectral theorem

In this section we will illustrate the usefulness of the spectral theorem. The most important topic for us is the decomposition of spectrum for unitary and self-adjoint operators. Spectral theorems for unitary and self-adjoint operators have the same character, to the extent that we will be able to discuss applications of the spectral theorem simultaneously for both cases.

Let T be a self-adjoint or unitary operator on $\mathcal{H}$. The spectral theorem establishes existence of a pair $(\{\mu_n\}_{n=1}^N, W)$ where the μ_n are probability measures on $\mathbb{C}$ and W is a unitary operator

$$W\colon \bigoplus_{n=1}^N L^2(\mathbb{C}, d\mu_n) \to \mathcal{H} \tag{1.9.1}$$

such that

$$D(T) = W\left(\left\{ f \in \bigoplus_{n=1}^N L^2(\mathbb{C}, d\mu_n) \,\middle|\, \sum_{n=1}^N \int |zf_n(z)|^2 d\mu_n(z) < \infty \right\}\right) \tag{1.9.2}$$

and for every $f \in \bigoplus_{n=1}^N L^2(\mathbb{C}, d\mu_n)$,

$$(W^{-1}TWf)_n(z) = zf_n(z) \tag{1.9.3}$$

Any such pair $(\{\mu_n\}_{n=1}^N, W)$ is called a *spectral representation* for T.

The only difference between the self-adjoint and unitary cases is that for a unitary operator, $\operatorname{supp}\mu_n \subset \partial\mathbb{D}$, and for a self-adjoint operator, $\operatorname{supp}\mu_n \subset \mathbb{R}$. We should note that there is a version of the spectral theorem for bounded normal operators, i.e. operators T with $TT^* = T^*T$, and for such operators the spectral measures can be supported on arbitrary compact sets in $\mathbb{C}$.

In our proof of the spectral theorem, there was a lot of freedom of choice when constructing the sequence $\{\psi_n\}_{n=1}^N$, so it is easy to see that the spectral representation is far from unique. For example, if two measures are mutually absolutely continuous, multiplications by z in the corresponding L^2 spaces are unitarily equivalent. We will skip the interesting topic of describing the set of possible spectral representations and finding a choice that is canonical in some sense and unique up to mutual absolute continuity, and we direct the reader to [49, Chapter VII] for more information.

Theorem 1.9.1. *Let T be a unitary or self-adjoint operator. The spectrum of T is given by*

$$\sigma(T) = \overline{\bigcup_{n=1}^N \operatorname{supp}\mu_n} \tag{1.9.4}$$

If T is self-adjoint, T is bounded if and only if for some $r > 0$, $\sigma(T) \subset [-r, r]$, in which case

$$\|T\| = \sup\big\{|x| \big| x \in \sigma(T)\big\} \tag{1.9.5}$$

Proof. This theorem follows directly from the fact that spectrum and norm of an operator are unitary invariants and from what we know about multiplication operators (Example 1.5.1). ☐

Remark 1.9.1. The closure in (1.9.4) is necessary only if $N = \infty$, otherwise $\bigcup_{n=1}^N \operatorname{supp}\mu_n$ is already closed. In particular, if T has a cyclic vector ψ, then

$$\sigma(T) = \operatorname{supp} \mu_\psi \tag{1.9.6}$$

In the remainder of this text, it will be very important to differentiate between different types of spectrum. Theorem 1.9.1 provides a first connection between spectrum and spectral measures, and one of our decompositions of spectrum will be in terms of spectral measures.

Any positive measure on $\mathbb{R}$ or $\partial\mathbb{D}$ has a Lebesgue decomposition

$$d\mu = d\mu_{\text{ac}} + d\mu_{\text{sc}} + d\mu_{\text{pp}}$$

where $d\mu_{\text{ac}}$ is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$ or $\partial\mathbb{D}$, μ_{sc} is singular continuous with respect to Lebesgue measure and μ_{pp} is a pure point measure. This and (1.9.4) inspire the decomposition of spectrum into the absolutely continuous, singular continuous and pure point parts.

Definition 1.9.1. If $(\{\mu_n\}_{n=1}^N, W)$ is a spectral representation of T, then the absolutely continuous, singular continuous and pure point spectra of T, denoted $\sigma_{\text{ac}}(T)$, $\sigma_{\text{sc}}(T)$ and $\sigma_{\text{pp}}(T)$, respectively, are defined by

$$\sigma_*(T) = \overline{\bigcup_{n=1}^N \operatorname{supp} \mu_{n,*}}$$

where $*$ stands for ac, sc, or pp.

Note that the three spectra need not be disjoint, but their union is all of $\sigma(T)$. We omit the proof of the important fact that this decomposition is independent of choice of spectral representation.

In Section 1.2, we discussed the problems involved with defining functions of operators. Using the spectral theorem, we can now provide a satisfactory definition.

Definition 1.9.2. Let T be a self-adjoint (or unitary) operator with a spectral representation $(\{\mu_n\}_{n=1}^N, W)$. For bounded Borel functions h on $\mathbb{R}$ (or $\mathbb{D}$), we define $h(T)$ by

$$(W^{-1}h(T)Wf)_n(z) = h(z)f_n(z)$$

(compare with (1.9.3)).

It can be shown that $h(T)$ is independent of the choice of spectral representation, and has good algebraic and analytic properties. For example, since e^{itx} is a bounded function of $x \in \mathbb{R}$ for $t \in \mathbb{R}$, we now have a definition of e^{itA}, and it is easy to see that e^{itA} is a unitary operator with all the properties we would hope for, for example $e^{itA}e^{isA} = e^{i(t+s)A}$.

In Section 1.8, we acknowledged a discrepancy in how we define cyclic subspaces for bounded versus unbounded operators. One of the definitions was not suitable for unbounded operators, but for bounded operators, we can now show that the two definitions give the same closures of cyclic subspaces.

Corollary 1.9.2. *If A is a bounded self-adjoint operator, then*

$$\overline{\operatorname{span}\{(A-z)^{-1}\psi \mid z \in \mathbb{C} \setminus \mathbb{R}\}} = \overline{\operatorname{span}\{A^n\psi \mid n \in \mathbb{N}_0\}}$$

Proof. Since A is bounded, the spectral measure μ_ψ is supported on a bounded interval. Using the spectral theorem, this becomes a trivial consequence of the fact that, by Weierstrass' theorem,

$$\overline{\operatorname{span}\{(x-z)^{-1} \mid z \in \mathbb{C} \setminus \mathbb{R}\}} = \overline{\operatorname{span}\{x^n \mid n \in \mathbb{N}_0\}} = L^2(\mathbb{R}, d\mu)$$

□

Chapter 2

Orthogonal polynomials

2.1 Introduction

In this chapter we will describe the basics of the spectral theory of orthogonal polynomials on the real line (OPRL) and orthogonal polynomials on the unit circle (OPUC). Our main goal is to describe the concepts and tools needed in the remainder of this thesis, and we will barely scratch the surface of this fascinating area of mathematics. For book-length treatments of the spectral theory of OPRL and OPUC, we refer the reader to [70, 23, 21, 14, 60, 61, 63].

Let μ be a positive Borel measure on $\mathbb{C}$. The measure μ is said to have finite moments if

$$\int_{\mathbb{C}} |z|^n d\mu(z) < \infty, \quad n = 0, 1, 2, \dots \tag{2.1.1}$$

If that is the case, the moments of μ are the finite quantities

$$c_n = \int_{\mathbb{C}} z^n d\mu(z) \tag{2.1.2}$$

If μ has finite moments, then all the monomials z^n are elements of $L^2(\mathbb{C}, d\mu)$. Are the monomials linearly independent? If not, there exists a nonzero polynomial $Q(z)$ which is μ-a.e. equal to 0. This implies that the support of μ is a subset of the set of zeros of Q, so a finite set. It is customary in spectral theory to refer to such measures as trivial, and to define *nontrivial measures* as measures whose support is an infinite set.

In the remainder of this text, *we consider only nontrivial measures with finite moments.* As we have established, for such measures $1, z, z^2, \dots$ are a linearly independent sequence in $L^2(\mathbb{C}, d\mu)$ (although not necessarily a basis). Applying the Gram–Schmidt process to this sequence yields the sequence $p_n(z)$ (denoted $p_n(z, d\mu)$ when there is danger of ambiguity) such that $p_n(z)$ has degree n, a positive leading coefficient and

$$\langle p_m, p_n \rangle = \int_{\mathbb{C}} \bar{p}_m(z) p_n(z) d\mu(z) = \delta_{m,n} \tag{2.1.3}$$

By the nature of the Gram–Schmidt process,

$$\text{span}\{p_0, p_1, \ldots, p_n\} = \text{span}\{1, z, \ldots, z^n\} \tag{2.1.4}$$

and then by (2.1.3),

$$\langle q, p_n \rangle = 0, \quad \text{ if } \deg q < n \tag{2.1.5}$$

Also note that if the measure is scaled by a constant, so are the polynomials,

$$p_n(z, \lambda d\mu) = \frac{1}{\sqrt{\lambda}} p_n(z, d\mu)$$

so we will usually assume that we are dealing with probability measures.

The study of orthogonal polynomials began with special classes of polynomials, associated with the names of Jacobi, Legendre, Chebyshev, Laguerre, Hermite. These classical polynomials were discovered in the 19th century as solutions to interpolation problems and to certain second-order differential equations. The reader may be familiar with some of these classical polynomials and with the fact that they obey second-order recurrence relations as well as second-order differential equations. Since orthogonality was of secondary importance, with their traditional definitions classical polynomials are orthogonal but typically not normalized with respect to a measure on $\mathbb{R}$.

However, it turns out that the second-order linear differential equations are unique to the classical polynomials, by a theorem of Bochner [5] (see also [31, Section 20.1]), but that a finite-order recurrence relation is a universal property for measures supported in $\mathbb{R}$ or $\partial\mathbb{D}$.

For the spectral theory of orthogonal polynomials, orthogonality and the recurrence relation are cornerstones of the theory, so spectral theory focuses on the two cases when the measure is supported in $\mathbb{R}$ or $\partial\mathbb{D}$, which are (up to an affine transformation) the only two cases for which a finite-order recurrence relation is known. The remainder of this text will focus on those two cases. Moreover, the focus of spectral theory is not on specific examples, but rather on general relations between properties of a measure and properties of the coefficients in the recurrence relations.

Nonetheless, there are interesting general results outside of $\mathbb{R}$ and $\partial\mathbb{D}$. As an example, and as conclusion to this section, we state without proof a general result of Fejér [18] about zeros of orthogonal polynomials.

Theorem 2.1.1 (Fejér [18]). *Let μ be a nontrivial probability measure on $\mathbb{C}$ and p_n its orthogonal polynomials. All the zeros of p_n lie in the convex hull of* $\operatorname{supp} d\mu$. *If, moreover,* $\operatorname{supp} d\mu$ *is compact,* *then no extreme point of the hull is a zero of* p_n, *and if* $\operatorname{supp} d\mu$ *is not a subset of a straight line, all zeros lie in the interior of the convex hull.*

2.2 Orthogonal polynomials on the real line (OPRL)

In this section we focus on the case $\operatorname{supp}\mu \subset \mathbb{R}$. Note that when $\operatorname{supp}\mu \subset \mathbb{R}$, the Gram–Schmidt process will produce polynomials $p_n(x)$ with real coefficients. Our first goal is to show that the p_n obey a three-term recursion relation.

Theorem 2.2.1. *Let* $\operatorname{supp}\mu \subset \mathbb{R}$. *Then the* $p_n(x)$ *satisfy the Jacobi recursion relation*

$$xp_n(x) = a_{n+1}p_{n+1}(x) + b_{n+1}p_n(x) + a_np_{n-1}(x), \quad \forall n \geq 0 \tag{2.2.1}$$

where $a_n > 0$, $b_n \in \mathbb{R}$ *and we use the convention* $a_0 = 0$. *Moreover, the leading coefficient of* p_n *is*

$$\gamma_n = \frac{1}{a_1 \dots a_n} \tag{2.2.2}$$

Definition 2.2.1. The coefficients $\{a_n, b_n\}_{n=1}^{\infty}$ appearing in (2.2.1) are called *Jacobi coefficients* of the measure μ.

Remark 2.2.1. We warn the reader that the notation for Jacobi coefficients isn't standardized. The letters a and b may be switched and the numbering may start from 1 rather than 0. The reader can always compare the form of (2.2.1) to check which convention is being used. One refers to the b_n as the diagonal Jacobi coefficients and to a_n as off-diagonal Jacobi coefficients.

Proof. Since $xp_n(x)$ is a polynomial of degree $n+1$, it is a linear combination of $p_0, p_1, \dots, p_{n+1}$. By Example 1.5.1, multiplication by x is self-adjoint in $L^2(\mathbb{R}, d\mu)$, so

$$\langle xp_n, p_j \rangle = \langle p_n, xp_j \rangle = 0, \quad \forall j \leq n-2$$

since p_n is orthogonal to polynomials of degree less than n. Thus,

$$xp_n(x) = a_{n+1}p_{n+1}(x) + b_{n+1}p_n(x) + c_{n+1}p_{n-1}(x)$$

Taking inner products with p_{n+1} and p_{n-1}, we get $a_{n+1} = \langle p_{n+1}, xp_n \rangle$ and $c_{n+1} = \langle p_{n-1}, xp_n \rangle$, so using reality of coefficients of the polynomials, $c_{n+1} = \int p_{n-1}xp_n d\mu = a_n$. Denoting by $\gamma_n > 0$ the leading coefficient of p_n, we know $xp_n(x) - \frac{\gamma_n}{\gamma_{n+1}}p_{n+1}(x)$ has degree at most n, so by (2.1.5),

$$a_n = \langle xp_n, p_{n+1} \rangle = \left\langle \frac{\gamma_n}{\gamma_{n+1}}p_{n+1}, p_{n+1} \right\rangle = \frac{\gamma_n}{\gamma_{n+1}} > 0$$

which by induction implies (4.4.36). The proof is concluded by $b_n = \langle xp_n, p_n\rangle = \int xp_n^2 d\mu \in \mathbb{R}$. □

We proceed by giving a few important examples.

Example 2.2.1. Chebyshev polynomials of the first kind, discovered in 1854 by Chebyshev [12, 13], are defined by the formula

$$T_n(\cos\theta) = \cos(n\theta) \tag{2.2.3}$$

They are orthogonal with respect to the probability measure $\frac{1}{\pi}\chi_{(-1,1)}(x)(1-x^2)^{-1/2}dx$,

$$\int_{-1}^{1} T_m(x)T_n(x)\frac{1}{\pi\sqrt{1-x^2}}dx = \begin{cases} 0, & m \neq n \\ 1, & m = n = 0 \\ 1/2, & m = n \neq 0 \end{cases}$$

by the standard change of variables $x = \cos\theta$. The orthonormal polynomials are given by $p_0(x) = 1$, $p_n(x) = \sqrt{2}T_n(x)$ for $n \geq 1$. By (2.2.1), we see $b_n \equiv 0$ and $a_1 = \frac{1}{\sqrt{2}}$, $a_n = \frac{1}{2}$ for $n \geq 2$.

Chebyshev polynomials were originally discovered for their property that of all monic polynomials P of degree n, $2^{-(n-1)}T_n(x)$ has the smallest $\| \|_\infty$-norm on $[-1,1]$ (equivalently, of all polynomials P of degree n for which $\sup_{-1\leq x\leq 1}|P(x)| \leq 1$, T_n has the largest leading coefficient).

Example 2.2.2. Chebyshev polynomials of the second kind are defined by the formula

$$U_n(\cos\theta) = \frac{\sin((n+1)\theta)}{\sin\theta} \tag{2.2.4}$$

They are orthonormal with respect to the probability measure $\frac{2}{\pi}\chi_{(-1,1)}(x)(1-x^2)^{1/2}dx$,

$$\frac{2}{\pi}\int_{-1}^{1} U_m(x)U_n(x)\sqrt{1-x^2}dx = \delta_{m,n}$$

From (2.2.1), we have $a_n \equiv \frac{1}{2}$ and $b_n \equiv 0$.

Our focus in this text will be on measures with

$$\lim_{n\to\infty} a_n = 1, \quad \lim_{n\to\infty} b_n = 0 \tag{2.2.5}$$

Thus, a special place in the theory will belong to the measure for which $a_n \equiv 1$ and $b_n \equiv 0$. We will refer to this measure as the "free case" for OPRL (by analogy with Schrödinger operators $-\Delta + V$ where the free case corresponds to $V \equiv 0$, i.e. the free Laplacian) and we will often think of measures with (2.2.5) as perturbations of the free case. It is thus of significant interest to find the explicit formula for this measure. We are about to find it: we just need to scale the measure from the previous example by a factor of 2. If $d\tilde{\mu}(x) = d\mu(x/\lambda)$, a linear change of variables on (2.1.3) gives

$$p_n(x, d\tilde{\mu}) = p_n(x/\lambda, d\mu)$$

and $a_n(d\tilde{\mu}) = \lambda a_n(d\mu)$, $b_n(d\tilde{\mu}) = \lambda b_n(d\mu)$. Thus, with $\lambda = 2$, we have

Example 2.2.3 (The "free case" for OPRL). Let

$$d\mu(x) = \frac{1}{2\pi}\chi_{(-2,2)}(x)\sqrt{4-x^2}\,dx \tag{2.2.6}$$

Orthonormal polynomials with respect to this measure are given by $p_n(x) = U_n(2x)$, and the corresponding Jacobi coefficients are $a_n \equiv 1$, $b_n \equiv 0$. Note that $d\mu$ is purely absolutely continuous and $\operatorname{supp} d\mu = [-2, 2]$.

In the preceding discussion, we seem to imply that the condition $a_n \equiv 1$, $b_n \equiv 0$ determines the measure uniquely. We will soon prove a theorem of Stieltjes [64] (but more commonly known as Favard's theorem) which asserts that this is indeed the case: if $\{a_n, b_n\}_{n=1}^\infty$ is a bounded sequence, it corresponds to a unique compactly supported measure. Note that for an unbounded sequence $\{a_n, b_n\}_{n=1}^\infty$, there may be more than one measure corresponding to those Jacobi parameters, and the problem of describing the set of such measures is known as the moment problem.

We will present a proof of Stieltjes' theorem which uses a certain class of tridiagonal matrices, known as Jacobi matrices. As we announced, our focus will be on bounded Jacobi parameters,

$$\sup_n a_n + \sup_n |b_n| < \infty \tag{2.2.7}$$

In the framework of unbounded operators, Jacobi matrices can still be defined when (2.2.7) is false, but we will have no need for unbounded Jacobi matrices in this text.

Definition 2.2.2. For a sequence $\{a_n, b_n\}_{n=1}^\infty$ with $a_n > 0$, $b_n \in \mathbb{R}$, and (2.2.7), a Jacobi matrix will be an operator on $\ell^2(\mathbb{N}_0)$, given by the formal expression

$$J(a,b) = \begin{pmatrix} b_1 & a_1 & & \\ a_1 & b_1 & a_2 & \\ & a_2 & b_2 & \ddots \\ & & \ddots & \ddots \end{pmatrix} \tag{2.2.8}$$

which is shorthand notation for saying that for any $u = \{u_n\}_{n=0}^\infty \in \ell^2(\mathbb{N}_0)$,

$$(J(a,b)u)_n = a_{n+1}u_{n+1} + b_{n+1}u_n + a_n u_{n-1} \tag{2.2.9}$$

As before, we use the convention $a_0 = 0$. The condition (2.2.7) implies that $J(a,b)u$ is indeed an element of $\ell^2(\mathbb{N}_0)$.

For $n \geq 0$, we denote by $\delta_n = (0, \dots, 0, 1, 0, \dots)$ the element of $\ell^2(\mathbb{N}_0)$ which has a single 1 as the n-th entry and 0 in all the other places. This is not to be confused with $\delta_{m,n}$, which is the Kronecker delta symbol, equal to 1 if $m = n$ and 0 otherwise.

Theorem 2.2.2. *(i) $J(a,b)$ is self-adjoint.*

(ii) δ_0 is a cyclic vector for $J(a,b)$ and the corresponding spectral measure has Jacobi coefficients $\{a_n, b_n\}_{n=1}^{\infty}$.

(iii) If two nontrivial compactly supported measures have the same Jacobi parameters, they are equal.

(iv) (Stieltjes) (2.2.1) *provides a bijection between compactly supported nontrivial probability measures on $\mathbb{R}$ and sequences $\{a_n, b_n\}_{n=1}^{\infty} \in (0,\infty)^\infty \times \mathbb{R}^\infty$ which satisfy* (2.2.7).

Proof. (i) This is a straightforward calculation, using the fact that $a_n, b_n \in \mathbb{R}$.

(ii) A direct calculation shows

$$J(a,b)^n \delta_0 - \Big(\prod_{j=1}^{n} a_j\Big)\delta_n \in \operatorname{span}\{\delta_k \mid 0 \leq k \leq n-1\}$$

and since $a_j \neq 0$, this implies that

$$\operatorname{span}\{J(a,b)^n \delta_0 \mid n \in \mathbb{N}_0\} = \operatorname{span}\{\delta_n \mid n \in \mathbb{N}_0\}$$

so δ_0 is a cyclic vector. Thus, there is a spectral measure μ_0 and a unitary map $W\colon L^2(\mathbb{R}, d\mu_0) \to \ell^2(\mathbb{N}_0)$ such that $W^{-1}J(a,b)W$ is multiplication by x on $L^2(\mathbb{R}, \mu_0)$ and $W1 = \delta_0$.

Define $p_n = W^{-1}\delta_n \in L^2(\mathbb{R}, d\mu_0)$. Since W is a unitary map,

$$\langle p_m, p_n \rangle = \langle \delta_m, \delta_n \rangle = \delta_{m,n} \tag{2.2.10}$$

Since $W^{-1}J(a,b)W$ is multiplication by x,

$$xp_n(x) = W^{-1}J(a,b)Wp_n(x) = W^{-1}J(a,b)\delta_n$$

But by definition of $J(a,b)$, this gives

$$xp_n(x) = W^{-1}(a_{n+1}\delta_{n+1} + b_{n+1}\delta_n + a_n\delta_{n-1}) = a_{n+1}p_{n+1} + b_{n+1}p_n + a_np_{n-1} \tag{2.2.11}$$

Since $p_0 = W^{-1} = 1$, this inductively implies that the p_n is a polynomial of degree n, and (2.2.10) tells us it is the n-th orthogonal polynomial of μ_0. Finally, (2.2.11) tells us the Jacobi parameters of μ_0 are $\{a_n, b_n\}_{n=1}^{\infty}$, as desired.

(iii) If μ and $\tilde{\mu}$ have the same Jacobi parameters, then by the Jacobi recursion relation, they have the same orthogonal polynomials p_n. Thus,

$$\int p_n d\mu = \langle 1, p_n \rangle_\mu = \delta_{n,0} = \langle 1, p_n \rangle_{\tilde{\mu}} = \int p_n d\tilde{\mu}$$

and then by linearity, $\int P d\mu = \int P d\tilde{\mu}$ for any polynomial P. The measures are supported in a compact set K and, by Weierstrass' theorem, polynomials are dense in $C(K)$, so this implies $\mu = \tilde{\mu}$.

(iv) This is immediate from (ii) and (iii). □

The final topic in this section is a result of Blumenthal–Weyl [4, 78]. We remind the reader that the essential support of a measure, denoted ess supp, is the support of the measure with any isolated points removed.

Theorem 2.2.3. *If* $a_n \to 1$, $b_n \to 0$, *then* $\operatorname{ess\,supp} \rho = [-2, 2]$.

Proof. Let us denote by $J^{(N)}$ the Jacobi matrix with coefficients

$$a_n^{(N)} = \begin{cases} a_n, & n \le N \\ 1, & n > N \end{cases}$$

$$b_n^{(N)} = \begin{cases} b_n, & n \le N \\ 0, & n > N \end{cases}$$

It is straightforward to see that $J^{(N)} - J^{(0)}$ is a finite rank operator and that $a_n \to 1$, $b_n \to 0$ implies $\|J^{(N)} - J(a,b)\| \to 0$, so $J(a,b) - J^{(0)}$ is a compact operator. Since $a_n \equiv 1$, $b_n \equiv 0$ corresponds to the measure (2.2.6), Weyl's theorem (Theorem 1.4.1) implies $\operatorname{ess\,supp} d\rho = [-2, 2]$. □

2.3 Orthogonal polynomials on the unit circle (OPUC)

In this section we study the case $\operatorname{supp} d\mu \subset \partial\mathbb{D}$. We will follow a common convention that orthogonal polynomials on the unit circle are denoted by φ_n instead of p_n.

The study of OPUC was initiated by Szegő [68, 69] in 1920 in connection with Toeplitz matrices. The recursion relation was first published by Szegő [70] in 1939, but the coefficients appearing in it were discovered earlier, in a different context; in 1933, Verblunsky [73] established the connection between these coefficients and the measure via the moments of the measure, an approach which we will not pursue in this text.

We begin by establishing that the polynomials obey a recursion relation. The recursion relation for OPUC turns out to be of a different form than the Jacobi recursion relation satisfied by OPRL. It will involve a polynomial

$$\varphi_n^*(z) = z^n \overline{\varphi_n(1/\bar{z})} \tag{2.3.1}$$

derived from $\varphi_n(z)$. Note that for $z \in \partial\mathbb{D}$, $\varphi_n^*(z) = z^n \overline{\varphi_n(z)}$ and that (2.1.5) implies

$$\langle z^k, \varphi_n^*(z) \rangle = \int z^{n-k} \bar{\varphi}_n(z) d\mu(z) = \langle \varphi_n(z), z^{n-k} \rangle = 0, \quad 1 \le k \le n \tag{2.3.2}$$

Theorem 2.3.1. *If* $\operatorname{supp} d\mu \subset \partial\mathbb{D}$, *orthonormal polynomials* φ_n *obey the Szegő recursion relation*

$$\varphi_{n+1}(z) = \frac{1}{\sqrt{1 - |\alpha_n|^2}} \big(z\varphi_n(z) - \bar{\alpha}_n \varphi_n^*(z) \big), \quad n \ge 0 \tag{2.3.3}$$

and the dual relation

$$\varphi_{n+1}^*(z) = \frac{1}{\sqrt{1 - |\alpha_n|^2}} \big(\varphi_n^*(z) - \bar{\alpha}_n z \varphi_n(z) \big), \quad n \ge 0 \tag{2.3.4}$$

where for $n \ge 0$, *the coefficients* α_n *satisfy* $|\alpha_n| < 1$ *and we use the convention* $\alpha_{-1} = -1$.

Definition 2.3.1. The coefficients $\{\alpha_n\}_{n=0}^\infty$ appearing in (2.3.3) are called *Verblunsky coefficients* of the measure μ.

Remark 2.3.1. We emphasize that the name and notation for Verblunsky coefficients are far from standard. They are referred to by several different names and denoted by different letters, and some authors' definition differs from ours by an extra complex conjugate or a different choice of sign. The reader can always compare the form of (2.3.3) to check which convention is being used. Our choice follows [60, 61].

Proof of Theorem 2.3.1. The idea is to show we can pick α_n such that

$$\langle \varphi_k, z\varphi_n - \bar{\alpha}_n \varphi_n^* \rangle = 0 \quad \text{for } 0 \le k \le n \tag{2.3.5}$$

Since $z = 1/\bar{z}$ for $z \in \operatorname{supp} d\mu \subset \partial\mathbb{D}$, for $1 \le k \le n$ we have $\langle z^k, z\varphi_n \rangle = \langle z^{k-1}, \varphi_n \rangle = 0$ and (2.3.2). Also note that $\langle 1, \varphi_n^* \rangle = \int z^n \bar{\varphi}_n(z) d\mu(z) = \langle \varphi_n(z), z^n \rangle \neq 0$, so we can define α_n by

$$\bar{\alpha}_n = \frac{\langle 1, z\varphi_n \rangle}{\langle 1, \varphi_n^* \rangle}$$

With this definition, $\langle z^k, z\varphi_n - \bar{\alpha}_n \varphi_n^* \rangle = 0$ for $0 \le k \le n$, so (2.3.5) holds by (2.1.4). Since $z\varphi_n - \bar{\alpha}_n \varphi_n^*$ is a polynomial of degree $n+1$, it is a linear combination of $\varphi_0, \varphi_1, \ldots, \varphi_{n+1}$. By

(2.3.5), it is a multiple of φ_{n+1}, so

$$z\varphi_n(z) = \rho_n\varphi_{n+1}(z) + \bar{\alpha}_n\varphi_n^*(z) \tag{2.3.6}$$

Now we note that $\|z\varphi_n\|^2 = \|\varphi_n\|^2 = 1$ and $\langle\varphi_n^*, \varphi_{n+1}\rangle = 0$ since φ_n^* has degree at most n. By computing the norms of both sides of (2.3.6), we get $1 = |\rho_n|^2 + |\alpha_n|^2$. Since the leading coefficients of $z\varphi_n$ and φ_{n+1} are strictly positive, we see that $\rho_n > 0$, so

$$\rho_n = \sqrt{1 - |\alpha_n|^2} \tag{2.3.7}$$

which concludes the proof. (2.3.4) follows directly from (2.3.3) by the definition of φ_n^*. □

It will be useful to keep the meaning of the letter ρ_n from the previous proof, as given by (2.3.7).

Let us note that (2.3.3) and (2.3.4) can be restated as saying that $\binom{\varphi_n(z)}{\varphi_n^*(z)}$ is the solution of the matrix recursion relation

$$\begin{pmatrix} \varphi_{n+1}(z) \\ \varphi_{n+1}^*(z) \end{pmatrix} = \frac{1}{\rho_n} \begin{pmatrix} z & -\bar{\alpha}_n \\ -\alpha_n z & 1 \end{pmatrix} \begin{pmatrix} \varphi_n(z) \\ \varphi_n^*(z) \end{pmatrix} \tag{2.3.8}$$

which corresponds to initial conditions $\binom{\varphi_n(z)}{\varphi_n^*(z)} = \binom{1}{1}$. One may try to analyze solutions of this matrix relation with arbitrary initial conditions, abandoning (2.3.1) and treating the two components of $\binom{\varphi_n(z)}{\varphi_n^*(z)}$ as independent. This is a valuable point of view, and we will see a glimpse of it in Section 2.5.

Example 2.3.1 (The "free case" for OPUC). Let

$$d\mu(e^{i\theta}) = \frac{d\theta}{2\pi}$$

be the Lebesgue measure on $\partial\mathbb{D}$. Since $\int_0^{2\pi} e^{in\theta}\frac{d\theta}{2\pi} = \delta_{n,0}$, the corresponding orthonormal polynomials are $\varphi_n(z) = z^n$. By (2.3.1) and (2.3.3), $\varphi_n^*(z) = 1$ and $\alpha_n \equiv 0$.

The previous theorem maps to each nontrivial measure μ a sequence of Verblunsky coefficients $\{\alpha_n\}_{n=0}^\infty \in \mathbb{D}^\infty$. By a theorem of Verblunsky [73], this map is a bijection. We will present a relatively modern proof of this fact, due to Simon [60, Section 4.2], which depends on the concept of CMV matrices. CMV matrices are a class of unitary matrices acting on $\ell^2(\mathbb{N}_0)$, named after Cantero–Moral–Velázquez [9] who established their connection with measures on the unit circle. In this sense, CMV matrices provide an appropriate analogue to Jacobi matrices.

The motivation for the definition of CMV matrices comes from the attempt to find an orthonormal basis for $L^2(\partial\mathbb{D}, d\mu)$ in which we can find an explicit matrix representation for multiplication by z. For OPRL, the polynomials themselves were often an orthonormal basis; for OPUC, not so much (it can in fact be proved that they are an orthonormal basis if and only if $\{\alpha_n\} \notin \ell^2$). However, Laurent polynomials are dense in $L^2(\partial\mathbb{D}, d\mu)$, so we can order the set of monomials as $1, z, z^{-1}, z^2, z^{-2}, \ldots$ and apply the Gram–Schmidt process. This gives an orthonormal basis denoted by $\{\chi_n(z)\}_{n=0}^{\infty}$, and the crucial discovery of Cantero–Moral–Velázquez is that χ_n can be expressed in terms of φ_n.

Denote by $P_{k,l}$ the orthogonal projection to the subspace $\operatorname{span}\{z^j \mid j \in \mathbb{Z}, k \leq j \leq l\}$ in $L^2(\partial\mathbb{D}, d\mu)$. Then the Gram–Schmidt process can be written as

$$\chi_{2n}(z) = \frac{z^{-n} - P_{-n+1,n} z^{-n}}{\|z^{-n} - P_{-n+1,n} z^{-n}\|} \tag{2.3.9}$$

$$\chi_{2n+1}(z) = \frac{z^{n+1} - P_{-n,n} z^{n+1}}{\|z^{n+1} - P_{-n,n} z^{n+1}\|} \tag{2.3.10}$$

Denote by U multiplication by z in $L^2(\partial\mathbb{D}, d\mu)$. Since U is unitary, one directly verifies

$$U^j P_{k,l} U^{-j} = P_{j+k,j+l}$$

so applying U^n to (2.3.9) and (2.3.10) gives

$$z^n \chi_{2n}(z) = \frac{1 - P_{1,2n} 1}{\|1 - P_{1,2n} 1\|} = \varphi_{2n}^*(z) \tag{2.3.11}$$

$$z^n \chi_{2n+1}(z) = \frac{z^{2n+1} - P_{0,2n} z^{2n+1}}{\|z^{2n+1} - P_{0,2n} z^{2n+1}\|} = \varphi_{2n+1}(z) \tag{2.3.12}$$

We have thus represented the basis $\{\chi_n\}_{n=0}^{\infty}$ in terms of the φ_n. The next step is to express $z\chi_n(z)$ in terms of χ_n. Using the Szegő recurrence, after some calculation we have

$$z\chi_{2n} = \rho_{2n-1}\rho_{2n-2}\chi_{2n-2} - \rho_{2n-1}\alpha_{2n-2}\chi_{2n-1} - \bar{\alpha}_{2n}\alpha_{2n-1}\chi_{2n} - \rho_{2n}\alpha_{2n-1}\chi_{2n+1} \tag{2.3.13}$$

$$z\chi_{2n+1} = \bar{\alpha}_{2n+1}\rho_{2n}\chi_{2n} - \bar{\alpha}_{2n+1}\alpha_{2n}\chi_{2n+1} + \bar{\alpha}_{2n+2}\rho_{2n+1}\chi_{2n+2} + \rho_{2n+2}\rho_{2n+1}\chi_{2n+3} \tag{2.3.14}$$

Replacing the χ_n with an orthonormal basis δ_n of $\ell^2(\mathbb{N}_0)$, we make the following definition.

Definition 2.3.2. For a sequence $\{\alpha_n\}_{n=0}^{\infty} \in \mathbb{D}^{\infty}$, the corresponding CMV matrix $\mathcal{C}(\alpha)$ is a five-diagonal matrix acting on $\ell^2(\mathbb{N}_0)$, given by

$$\mathcal{C}(\alpha) = \begin{pmatrix} \bar{\alpha}_0 & \bar{\alpha}_1\rho_0 & \rho_1\rho_0 & & & \\ \rho_0 & -\bar{\alpha}_1\alpha_0 & -\rho_1\alpha_0 & & & \\ & \bar{\alpha}_2\rho_1 & -\bar{\alpha}_2\alpha_1 & \bar{\alpha}_3\rho_2 & \rho_3\rho_2 & \\ & \rho_2\rho_1 & -\rho_2\alpha_1 & -\bar{\alpha}_3\alpha_2 & -\rho_3\alpha_2 & \ddots \\ & & & \bar{\alpha}_4\rho_3 & -\bar{\alpha}_4\alpha_3 & \ddots \\ & & & \ddots & \ddots & \ddots \end{pmatrix} \tag{2.3.15}$$

Put differently, this is the matrix on $\ell^2(\mathbb{N}_0)$ which acts on basis vectors δ_n as follows,

$$\mathcal{C}(\alpha)\delta_{2n} = \rho_{2n-1}\rho_{2n-2}\delta_{2n-2} - \rho_{2n-1}\alpha_{2n-2}\delta_{2n-1} - \bar{\alpha}_{2n}\alpha_{2n-1}\delta_{2n} - \rho_{2n}\alpha_{2n-1}\delta_{2n+1} \tag{2.3.16}$$

$$\mathcal{C}(\alpha)\delta_{2n+1} = \bar{\alpha}_{2n+1}\rho_{2n}\delta_{2n} - \bar{\alpha}_{2n+1}\alpha_{2n}\delta_{2n+1} + \bar{\alpha}_{2n+2}\rho_{2n+1}\delta_{2n+2} + \rho_{2n+2}\rho_{2n+1}\delta_{2n+3} \tag{2.3.17}$$

(with the convention $\alpha_{-1} = -1$, and thus $\rho_{-1} = 0$, as before).

Since $\alpha_n, \rho_n \in \mathbb{D}$, (2.3.16) and (2.3.17) give $\|\mathcal{C}(\alpha)\delta_n\| \leq 4$. Since $\langle \mathcal{C}\delta_m, \mathcal{C}\delta_n\rangle = 0$ when $|m-n| \geq 5$,

$$\left|\left\langle \sum_{m\in\mathbb{Z}} \beta_m \mathcal{C}\delta_m, \sum_{n\in\mathbb{Z}} \beta_n \mathcal{C}\delta_n \right\rangle\right| \leq \sum_{n\in\mathbb{Z}} \sum_{k=-4}^{4} \bar{\beta}_{n+k}\beta_n \|C\delta_{n+k}\| \, \|C\delta_n\| \leq \sum_{k=-4}^{4} 16 \sum_{n\in\mathbb{Z}} |\beta_n|^2 = 144 \left\| \sum_{n\in\mathbb{Z}} \beta_n \delta_n \right\|^2$$

(with Cauchy–Schwarz applied in the last step), the previous definition clearly constructs a well-defined, bounded operator $\mathcal{C}$ with $\|\mathcal{C}\| \leq 12$. We will soon discover that $\mathcal{C}$ is in fact unitary!

Note that if $\{\alpha_n\}_{n=0}^\infty$ are the Verblunsky coefficients of a measure μ, then comparing (2.3.13), (2.3.14) with (2.3.16), (2.3.17), we see that $\mathcal{C}(\alpha)$ is multiplication by z in $L^2(\partial\mathbb{D}, d\mu)$ in the basis $\{\chi_n\}_{n=0}^\infty$.

We now establish some properties of $\mathcal{C}(\alpha)$, culminating in a proof of Verblunsky's theorem [73].

Theorem 2.3.2. *(i) $\mathcal{C}(\alpha)$ is unitary.*

(ii) δ_0 is a cyclic vector for $\mathcal{C}(\alpha)$ and its spectral measure has Verblunsky coefficients $\{\alpha_n\}_{n=0}^\infty$.

(iii) A probability measure on $\partial\mathbb{D}$ is uniquely determined by its Verblunsky coefficients.

(iv) (Verblunsky) (2.3.3) provides a bijection between nontrivial probability measures on $\partial\mathbb{D}$ and sequences $\alpha = \{\alpha_n\}_{n=0}^\infty \in \mathbb{D}^\infty$.

The ideas of the proof are the same as in the proof of Theorem 2.2.2, but the realization is somewhat more cumbersome because of the more complicated form of CMV matrices.

Proof. (i) This follows directly from the (non-obvious but straightforward to check) observation that

$$\mathcal{C}(\alpha) = \begin{pmatrix} \Theta_0 & & & \\ & \Theta_2 & & \\ & & \Theta_4 & \\ & & & \ddots \end{pmatrix} \begin{pmatrix} 1 & & & \\ & \Theta_1 & & \\ & & \Theta_3 & \\ & & & \ddots \end{pmatrix} \tag{2.3.18}$$

where 1 stands for a single entry of 1 and Θ_j are unitary 2×2 matrices

$$\Theta_j = \begin{pmatrix} \bar{\alpha}_j & \rho_j \\ \rho_j & -\alpha_j \end{pmatrix} \tag{2.3.19}$$

(ii) From (2.3.15),

$$(\mathcal{C}^*)^n\delta_0 - \prod_{k=0}^{2n-1} \rho_k \delta_{2n} \in \operatorname{span}\{\delta_k \mid 0 \le k \le 2n-1\}, \quad n \ge 0$$
$$\mathcal{C}^n\delta_0 - \prod_{k=0}^{2n-2} \rho_k \delta_{2n-1} \in \operatorname{span}\{\delta_k \mid 0 \le k \le 2n-2\}, \quad n \ge 1$$

so since $\rho_k > 0$, $\mathcal{C}^* = \mathcal{C}^{-1}$, and $\langle \delta_m, \delta_n \rangle = \delta_{m,n}$, the sequence $\{\delta_n\}_{n=0}^\infty$ is the result of the Gram–Schmidt process applied to the sequence δ_0, $\mathcal{C}\delta_0$, $\mathcal{C}^{-1}\delta_0$, $\mathcal{C}^2\delta_0$, $\mathcal{C}^{-2}\delta_0$, ...

Thus, δ_0 is a cyclic vector and we have a unitary map $W\colon L^2(\partial\mathbb{D}, d\mu_0) \to \ell^2(\mathbb{N}_0)$ such that $W1 = \delta_0$ and $W^{-1}\mathcal{C}W$ is multiplication by z in $L^2(\partial\mathbb{D}, \mu_0)$. Thus, $Wz^n = \mathcal{C}^n\delta_0$ for $n \in \mathbb{Z}$.

Defining $\chi_n = W^{-1}\delta_n \in L^2(\mathbb{C}, d\mu_0)$ for $n \in \mathbb{N}_0$, since W is a unitary map, $\{\chi_n\}_{n=0}^\infty$ is the result of the Gram–Schmidt process applied to

$$\langle \chi_m, \chi_n \rangle = \langle \delta_m, \delta_n \rangle = \delta_{m,n} \tag{2.3.20}$$

so it is just the usual basis for $L^2(\partial\mathbb{D}, d\mu_0)$ as defined in (2.3.9), (2.3.10). Denoting the Verblunsky coefficients of μ_0 by α_n' and using the unitary map W to compare those coefficients, appearing in (2.3.13), (2.3.14), with the α_n appearing in (2.3.16), (2.3.17), we see that

$$\bar\alpha_n'\alpha_{n-1}' = \bar\alpha_n\alpha_{n-1}, \quad n \ge 0 \tag{2.3.21}$$
$$\rho_n'\rho_{n-1}' = \rho_n\rho_{n-1}, \quad n \ge 1 \tag{2.3.22}$$
$$\bar\alpha_n'\rho_{n-1}' = \bar\alpha_n\rho_{n-1}, \quad n \ge 1 \tag{2.3.23}$$

From $\alpha_{-1} = \alpha_{-1}' = -1$ and (2.3.21) we conclude $\alpha_0' = \alpha_0$ and thus $\rho_0' = \rho_0 \in (0, 1]$. Thus, induction with (2.3.22) implies $\rho_n' = \rho_n \in (0, 1]$ for all n, and finally, (2.3.23) implies $\alpha_n' = \alpha_n$.

(iii) From (2.3.13) and (2.3.14), if μ and $\tilde\mu$ have the same Verblunsky coefficients, then they have the same basis χ_n, so

$$\int \chi_n d\mu = \langle 1, \chi_n \rangle_\mu = \delta_{n,0} = \langle 1, \chi_n \rangle_{\tilde\mu} = \int \chi_n d\tilde\mu$$

and then by linearity, $\int Q d\mu = \int Q d\tilde\mu$ for any Laurent polynomial Q. Since Laurent polynomials are dense in $C(\partial\mathbb{D})$, this implies $\mu = \tilde\mu$.

(iv) This is an immediate corollary of (ii) and (iii). □

As the final topic in this section, we present a result of Geronimus [22, Theorem 19.1].

Theorem 2.3.3 (Geronimus)**.** *If* $\lim\limits_{n\to\infty} \alpha_n = 0$*, then* $\operatorname{supp} d\mu = \partial\mathbb{D}$.

Proof. Let $\mathcal{C}^{(N)}$ be the CMV matrix corresponding to the $\alpha^{(N)}$ defined by

$$\alpha_n^{(N)} = \begin{cases} \alpha_n, & n < N \\ 0, & n \geq N \end{cases} \tag{2.3.24}$$

In particular, $\mathcal{C}^{(0)}$ corresponds to $\alpha_n^{(0)} \equiv 0$. It is immediate from the definition that $\mathcal{C}^{(N)} - \mathcal{C}^{(0)}$ is finite rank,

$$\operatorname{Ran}(\mathcal{C}^{(N)} - \mathcal{C}^{(0)}) \subset \operatorname{span}\{\delta_k \mid 0 \leq k \leq N+2\}$$

Since $\alpha_n \to 0$ implies $\|\mathcal{C}^{(N)} - \mathcal{C}\| \to 0$, we conclude that $\mathcal{C} - \mathcal{C}^{(0)}$ is compact and Weyl's theorem (Theorem 1.4.1) implies $\sigma_{\text{ess}}(\mathcal{C}) = \sigma_{\text{ess}}(\mathcal{C}^{(0)})$. Since $\alpha_n^{(0)} \equiv 0$ corresponds to the measure $\frac{d\theta}{2\pi}$ (see Example 2.3.1), this implies $\operatorname{supp} d\mu = \partial\mathbb{D}$. □

Simon [60, Section 4.3] has an extension of this result: if $\lim_{n\to\infty}(\alpha_n - \beta_n) = 0$, then the corresponding measures μ and ν have equal essential supports (supports with isolated points removed).

2.4 Locating the a.c. spectrum in OPRL

In this section we will discuss two criteria for describing the absolutely continuous part of a measure ρ on $\mathbb{R}$. The first criterion will be in terms of a sequence of weak approximations to ρ, and this criterion will be useful for proving purely absolutely continuous spectrum on intervals. The second criterion is more sophisticated and will be useful in situations where absolutely continuous spectrum may be mixed with singular spectrum. We will also introduce Prüfer variables for OPRL.

The key to the first criterion is a sequence of weak approximations to $d\rho$, due to Simon [62]. This and similar approximations are usually referred to as "Carmona-type" approximations, honoring similar results by Carmona [11] for Schrödinger operators.

Theorem 2.4.1 (Simon [62]). *The sequence of measures* $\frac{dx}{\pi(a_n^2 p_n^2(x) + p_{n-1}^2(x))}$ *converges weakly to* $d\rho(x)$*, i.e. for bounded continuous functions* f *on* $\mathbb{R}$*,*

$$\lim_{n\to\infty} \int f(x) \frac{dx}{\pi(a_n^2 p_n^2(x) + p_{n-1}^2(x))} = \int f(x) d\rho(x) \tag{2.4.1}$$

We wish to state the next result in terms of Prüfer variables, so we must define them first. Prüfer variables are named after Prüfer [48], who defined them for Sturm–Liouville operators. The OPRL version of Prüfer variables is known as the EFGP transform, by Eggarter, Figotin, Gredeskul, Pastur [16, 27, 46] who developed and used it in the discrete Schrödinger case $a_n = 1$. It was also extensively used by Kiselev–Last–Simon [38]. For general OPRL, it was used by Breuer, Kaluzhny, Last, Simon [35, 6, 7, 8].

For $x \in (-2,2)$ parametrized as $x = 2\cos(\eta/2)$ by $\eta \in (0, 2\pi)$, define $r_n(x) > 0$, $\theta_n(x) \in \mathbb{R}$ by

$$r_n(x) e^{i[n\eta/2 + \theta_n(x)]} = a_n p_n(x) - p_{n-1}(x) e^{-i\eta/2} \tag{2.4.2}$$

Let us first note that (2.4.2) is nonzero, so this definition is valid: if the right-hand side of (2.4.2) was equal to 0, this would imply $p_n(x) = p_{n-1}(x) = 0$ by reality of $p_n(x)$, and then a reverse induction using the Jacobi recursion relation (2.2.1) would imply $p_n(x) = 0$ for all n, a contradiction with $p_0(x) = 1$.

We now define

$$\alpha_n(x) = \frac{a_n^2 - 1 + e^{i\eta/2} b_{n+1}}{e^{i\eta} - 1} \tag{2.4.3}$$

This variable provides a combination of a_n and b_n that is natural in this context, and will play the same role that Verblunsky coefficients α_n play for OPUC. In fact, after this section, we will not need to mention a_n or b_n individually, only their combination (2.4.3).

Multiplying (2.4.2) by $e^{i\eta/2}$ gives

$$r_n e^{i[(n+1)\eta/2 + \theta_n]} = a_n p_n e^{i\eta/2} - p_{n-1} \tag{2.4.4}$$

Note that $2\operatorname{Re}\alpha_n = 1 - a_n^2$ and $2\operatorname{Re}(\alpha_n e^{i\eta/2}) = b_{n+1}$ so using (2.4.4),

$$\begin{aligned} 2\operatorname{Re}\bigl(r_n e^{i[(n+1)\eta/2+\theta_n]} \alpha_n\bigr) &= 2\operatorname{Re}\bigl(a_n p_n e^{i\eta/2} \alpha_n - p_{n-1}\alpha_n\bigr) \\ &= a_n p_n b_{n+1} + (a_n^2 - 1) p_{n-1} \end{aligned}$$

Subtracting this from (2.4.4), then using the Jacobi recursion relation (2.2.1), we have

$$\begin{aligned} r_n e^{i[(n+1)\eta/2+\theta_n]} - 2\operatorname{Re}\bigl(r_n e^{i[(n+1)\eta/2+\theta_n]} \alpha_n\bigr) &= a_n (a_{n+1} p_{n+1} - p_n e^{-i\eta/2}) \\ &= a_n r_{n+1} e^{i[(n+1)\eta/2 + \theta_{n+1}]} \end{aligned}$$

where for the last step we used (2.4.2) with n replaced by $n+1$. Dividing by $a_n r_n e^{i[(n+1)\eta/2+\theta_n]}$ on both sides and again using $a_n^2 = 1 - 2\operatorname{Re}\alpha_n$, we get

$$\frac{r_{n+1}}{r_n} e^{i(\theta_{n+1} - \theta_n)} = \frac{1 - \alpha_n - \bar\alpha_n e^{-i[(n+1)\eta + 2\theta_n]}}{\sqrt{1 - \alpha_n - \bar\alpha_n}} \tag{2.4.5}$$

Multiplying or dividing this equation by its complex conjugate, we compute

$$\frac{r_{n+1}}{r_n} = \frac{|1 - \alpha_n - \bar\alpha_n e^{-i[(n+1)\eta + 2\theta_n]}|}{\sqrt{1 - \alpha_n - \bar\alpha_n}} \tag{2.4.6}$$

$$e^{2i(\theta_{n+1} - \theta_n)} = \frac{1 - \alpha_n - \bar\alpha_n e^{-i[(n+1)\eta + 2\theta_n]}}{1 - \bar\alpha_n - \alpha_n e^{i[(n+1)\eta + 2\theta_n]}} \tag{2.4.7}$$

In essence, we have traded the Jacobi recursion relation for a system of two first-order recursion relations (2.4.6), (2.4.7). The usefulness of this system comes partly from the fact that (2.4.7) is a decoupled relation with no dependence on r_n. Note also that if $a_n = 1$, $b_n = 0$, then $\alpha_n = 0$, so (2.4.5) implies $\theta_{n+1} = \theta_n$. We will use Prüfer variables to analyze perturbations around the free case, so it is convenient for us that when a_n and b_n are "close" to 1 and 0 respectively, θ_n varies slowly in some sense.

The following lemma provides a criterion for the measure ρ to have purely a.c. spectrum on an interval. This will be the basic criterion we will use in Chapter 4. Part (iii) of the lemma will be crucial for a proof by contradiction in Chapter 4.

Lemma 2.4.2. *Let a measure $d\rho = f(x)dx + d\rho_{\mathrm{s}}$ on $\mathbb{R}$ have Jacobi parameters $\{a_n, b_n\}_{n=1}^{\infty}$ with $a_n \to 1$, $b_n \to 0$ and Prüfer variables $r_n(x)$.*

(i) If $\log r_n(x)$ converges uniformly on an interval $I \subset (-2+\epsilon, 2-\epsilon)$ where $\epsilon > 0$, then

$$\chi_I(x)d\rho(x) = \chi_I(x)\frac{1}{2\pi}\frac{\sqrt{4-x^2}}{\lim\limits_{n\to\infty} r_n^2(x)}\,dx \tag{2.4.8}$$

so the measure ρ is purely absolutely continuous on I and $f(x)$ is continuous and strictly positive on I.

(ii) If $S \subset (-2,2)$ is finite and $\log r_n(x)$ converges uniformly on intervals $I \subset (-2,2)$ with $\mathrm{dist}(I, S \cup \{-2,2\}) > 0$, then $\mathrm{supp}\,\rho_{\mathrm{s}} \cap (-2,2) \subset S$ and $f(x)$ is continuous and strictly positive on $(-2,2) \setminus S$.

(iii) It is not possible for $\log r_n(x)$ to converge as $n \to \infty$ to $+\infty$ or $-\infty$ uniformly on an interval $I \subset (-2,2)$.

Proof. (i) We wish to use (2.4.1), but instead of control over $a_n^2 p_n^2 + p_{n-1}^2$, we only know that

$$r_n^2(x) = a_n^2 p_n^2(x) - a_n x p_n(x) p_{n-1}(x) + p_{n-1}^2(x) \tag{2.4.9}$$

converges uniformly on I. For $|x| < 2 - 2\epsilon$ we have

$$\epsilon(a_n^2 p_n^2(x) + p_{n-1}^2(x)) \le r_n^2(x) \le (2-\epsilon)(a_n^2 p_n^2(x) + p_{n-1}^2(x)) \tag{2.4.10}$$

Since $\log r_n$ converges uniformly on I, it is uniformly bounded on I, so (2.4.10) implies $\log(a_n^2 p_n^2(x) + p_{n-1}^2(x))$ is uniformly bounded on I. Thus, standard measure theory arguments applied to (2.4.1) imply that $\chi_I(x)d\rho(x) = \chi_I(x)f(x)dx$ with $\log f$ bounded on J.

It remains to prove continuity of f on I. By a result of Nevai [43, Theorem 4.2.13], since $a_n \to 1$

and $b_n \to 0$, for all bounded continuous real functions $h(x)$

$$\lim_{n\to\infty} \int_{-\infty}^{+\infty} h(x)p_n(x)p_{n+k}(x)d\rho(x) = \frac{1}{\pi}\int_{-2}^{2} h(x)\frac{T_{|k|}(x/2)}{\sqrt{4-x^2}}\,dx$$

where $T_k(x)$ are Chebyshev polynomials of the first kind, defined in Example 2.2.1. Using this and (2.4.9),

$$\lim_{n\to\infty} \int_{-\infty}^{+\infty} h(x)r_n(x)^2 d\rho(x) = \frac{1}{\pi}\int_{-2}^{2} h(x)\frac{2T_0(x/2) - xT_1(x/2)}{\sqrt{4-x^2}}\,dx \tag{2.4.11}$$

$$= \frac{1}{2\pi}\int_{-2}^{2} h(x)\sqrt{4-x^2}\,dx \tag{2.4.12}$$

If in addition $\operatorname{supp} h \subset I$, uniform convergence of $\log r_n(x)$ on I implies

$$\lim_{n\to\infty} \int_{-\infty}^{+\infty} h(x)r_n^2(x)\,d\rho(x) = \int_{-\infty}^{+\infty} h(x) \lim_{n\to\infty} r_n^2(x)\,d\rho(x) \tag{2.4.13}$$

Comparing (2.4.12) and (2.4.13) gives (2.4.8).

(ii) Since S is finite, $(-2,2)\setminus S$ can be covered by countably many intervals I which satisfy the conditions of (i), so (ii) follows from (i).

(ii) If $r_n(x)$ converged uniformly to 0 or to ∞ on I, (2.4.10) and (2.4.1) would imply that $\rho(I) = \infty$ or $\rho(I) = 0$. This would contradict either the assumption that $d\rho$ is a probability measure or Theorem 2.2.3. $\square$

We will now show an application of this criterion.

Theorem 2.4.3 (Titchmarsh)**.** *If a measure ρ has Jacobi coefficients $\{a_n, b_n\}_{n=1}^{\infty}$ with*

$$\sum_{n=1}^{\infty}|a_n - 1| + \sum_{n=1}^{\infty}|b_n| < \infty \tag{2.4.14}$$

and $a_n \to 1$, $b_n \to 0$, then $d\rho = f\,dx + d\rho_s$ is purely absolutely continuous on $(-2,2)$ and f is continuous and strictly positive on $(-2,2)$.

Proof. Taking the real part of the logarithm of (2.4.6), we see

$$\log\frac{r_{n+1}(x)}{r_n(x)} = \operatorname{Re}\log(1 - \alpha_n - \bar{\alpha}_n e^{-i[(n+1)\eta + 2\theta_n]}) - \tfrac{1}{2}\log(1 - \alpha_n - \bar{\alpha}_n) = O(|\alpha_n|)$$

By (2.4.3) and (2.4.14), on $I = (-2+\epsilon, 2-\epsilon)$, $\alpha_n(x)$ is uniformly ℓ^1. Thus, there exists a constant C independent of n or x such that

$$|\log r_{n+1}(x) - \log r_n(x)| \le C|\alpha_n(x)| \tag{2.4.15}$$

Since $\log r_1(x)$ is continuous in x, summing (2.4.15) over n shows that the sequence $\log r_n(x)$ converges uniformly on I, so all the conclusions follow from Lemma 2.4.2(i). □

For the second criterion we wish to present, we must look at formal eigensolutions of the Jacobi matrix, that is, sequences $\{u_n\}_{n=0}^{\infty}$ with

$$a_{n+1}u_{n+1} + b_{n+1}u_n + a_n u_{n-1} = xu_n \tag{2.4.16}$$

We emphasize that these are only formal eigensolutions because they need not be elements of $\ell^2(\mathbb{N}_0)$. Of course, for a fixed x, the set of solutions of (2.4.16) is a two-dimensional vector space. We will be interested in solutions which are, in a certain sense, asymptotically small compared to other solutions.

Definition 2.4.1. A solution $u = \{u_n\}_{n=0}^{\infty}$ of (2.4.16) is *subordinate* if for any linearly independent solution $v = \{v_n\}_{n=0}^{\infty}$,

$$\lim_{N\to\infty} \frac{\sum_{n=0}^{N}|u_n|^2}{\sum_{n=0}^{N}|v_n|^2} = 0 \tag{2.4.17}$$

The notion that (non)existence of subordinate solutions indicates the type of spectrum was discovered by Gilbert–Pearson [25], who developed subordinacy theory for Schrödinger operators on the half-line. The approach was extended by Gilbert [24] to the real line and by Khan–Pearson [37] to OPRL. Important contributions are due to Jitomirskaya–Last [33, 34], and a related criterion is due to Last–Simon [41].

Theorem 2.4.4 (Gilbert–Pearson)**.** *Let $d\rho = f\,dx + d\rho_{\mathrm{s}}$ be a probability measure on $\mathbb{R}$ with Jacobi parameters $\{a_n, b_n\}_{n=1}^{\infty}$, and let N be the set of $x \in \mathbb{R}$ for which there is no subordinate solution. The set N is an essential support for the absolutely continuous part of the measure ρ, and $\rho_{\mathrm{s}}(N) = 0$.*

For a proof, we direct the reader to [37] or [71, Section 3.3].

2.5 Locating the a.c. spectrum in OPUC

In this section we will discuss two criteria for describing the absolutely continuous part of a measure μ on $\partial\mathbb{D}$. The first criterion will be in terms of a sequence of weak approximations to μ, and this criterion will be useful for proving purely absolutely continuous spectrum on intervals. The second criterion is more sophisticated and involves solutions to the matrix recursion relation (2.3.8). It will be useful for proving existence of absolutely continuous spectrum even in situations where it may be mixed with singular spectrum. We will also introduce Prüfer variables for OPUC.

We start with a fact about measures with finitely many nonzero Verblunsky coefficients.

Theorem 2.5.1. *Let $\alpha_n = 0$ for $n \geq N$. Then $\varphi_n(z) = z^{n-N}\varphi_N(z)$ for $n > N$ and*

$$d\mu = \frac{1}{|\varphi_N(e^{i\theta})|^2} \frac{d\theta}{2\pi} \tag{2.5.1}$$

Proof. The first claim follows directly from the Szegő recursion (2.3.3). To show that the measure has the given form, we need a very mild fact that φ_n has no zeros on $\partial\mathbb{D}$ (in fact, φ_n has no zeros on $\mathbb{C} \setminus \mathbb{D}$, by Theorem 2.1.1). To prove this fact, assume that $\varphi_{n+1}(z) = 0$ for some z with $|z| = 1$. Then (2.3.3) gives $z\varphi_n(z) = \bar{\alpha}_n \varphi_n^*(z)$, but $|\alpha_n| < 1$ and $\varphi_n^*(z) = z^n \overline{\varphi_n(1/\bar{z})} = z^n \overline{\varphi_n(z)}$ mean that this is possible only if $\varphi_n(z) = 0$. Using this reasoning inductively, we conclude that $\varphi_k(z) = 0$ for all $k < n$, but since $\varphi_0(z) = 1$, we have reached a contradiction.

We now know that $|\varphi_N(e^{i\theta})|^2$ is a nonvanishing continuous function, so proving (2.5.1) is equivalent to proving $|\varphi_N(e^{i\theta})|^2 d\mu = \frac{d\theta}{2\pi}$. Integrating both measures against z^n, $n \in \mathbb{Z}$,

$$\int z^n |\varphi_N(e^{i\theta})|^2 d\mu = \langle \varphi_N(z), z^n \varphi_N(z) \rangle_\mu = \langle \varphi_N(z), \varphi_{N+n}(z) \rangle_\mu = \delta_{n,0}, \quad n \geq 0$$
$$\int z^n |\varphi_N(e^{i\theta})|^2 d\mu = \langle z^{-n} \varphi_N(z), \varphi_N(z) \rangle_\mu = \langle \varphi_{N-n}(z), \varphi_N(z) \rangle_\mu = 0, \qquad n < 0$$

and $\int e^{in\theta} \frac{d\theta}{2\pi} = \delta_{n,0}$, so the two measures are equal by density of Laurent polynomials. □

We can now establish a sequence of weak approximations to $d\mu$, in the form of measures with finitely many nonzero Verblunsky coefficients.

Theorem 2.5.2 (Bernstein–Szegő approximations)**.** *The measures $d\mu^{(N)} = \frac{1}{|\varphi_N(z)|^2} \frac{d\theta}{2\pi}$ weakly converge to the measure μ, i.e.*

$$\int f d\mu^{(N)} \to \int f d\mu, \quad \forall f \in C(\partial\mathbb{D})$$

Proof. Theorem 2.5.1 establishes that $\mu^{(N)}$ has coefficients $\alpha^{(N)}$ given by

$$\alpha_n^{(N)} = \begin{cases} \alpha_n, & n < N \\ 0, & n \geq N \end{cases} \tag{2.5.2}$$

Using the Szegő recursion inductively in n, we see that $\varphi_n^{(N)} = \varphi_n$ for $n \leq N$. Integrating φ_n and $\bar{\varphi}_n$ against $d\mu$ and $d\mu^{(N)}$, an induction in $|n|$ proves that $\int z^n d\mu^{(N)}(z) = \int z^n d\mu(z)$ for $|n| \leq N$. Since the $\mu^{(N)}$ and μ are probability measures and Laurent polynomials are dense in $C(\partial\mathbb{D})$, this completes the proof. □

Bernstein–Szegő approximations will provide the first criterion we announced. However, we wish to state this criterion in terms of Prüfer variables, so we must introduce them first. The OPUC version of Prüfer variables was first introduced by Nikishin [45], and their usefulness to spectral theory was exploited by Nevai [44] and Simon [61].

For $z = e^{i\eta}$ with $\eta \in \mathbb{R}$, Prüfer variables $r_n(z)$, $\theta_n(z)$ are defined by $r_n(z) > 0$, $\theta_n(z) \in \mathbb{R}$, and

$$\varphi_n(z) = r_n(z) e^{i[n\eta + \theta_n(z)]} \tag{2.5.3}$$

In the proof of Theorem 2.5.1, we have already shown that φ_n has no zeros on $\partial\mathbb{D}$, so $r_n > 0$, $\theta_n \in \mathbb{R}$ satisfying (2.5.3) do exist. The ambiguity in θ_n modulo 2π is usually fixed by setting $\theta_0 = 0$ and $|\theta_{n+1} - \theta_n| < \pi$, but in this text that will be irrelevant. Notice that (2.5.3) is in essence just the polar decomposition of $\varphi_n(z)$, except for the addition of the factor $e^{in\eta} = z^n$, which we will motivate shortly.

From (2.3.1) and (2.5.3), we have $\varphi_n^*(z) = r_n(z) e^{-i\theta_n(z)}$ so from the Szegő recursion relation,

$$r_n e^{i[(n+1)\eta + \theta_n]} = \sqrt{1 - |\alpha_n|^2}\, r_{n+1} e^{i[(n+1)\eta + \theta_{n+1}]} + \bar{\alpha}_n r_n e^{-i\theta_n}$$

Regrouping and dividing by $\sqrt{1 - |\alpha_n|^2}\, r_n e^{i[(n+1)\eta + \theta_n]}$ gives

$$\frac{r_{n+1}}{r_n} e^{i(\theta_{n+1} - \theta_n)} = \frac{1 - \bar{\alpha}_n e^{-i[(n+1)\eta + 2\theta_n]}}{\sqrt{1 - |\alpha_n|^2}} \tag{2.5.4}$$

Multiplying or dividing this equation by its complex conjugate, we compute

$$\frac{r_{n+1}}{r_n} = \frac{|1 - \alpha_n e^{i[(n+1)\eta + 2\theta_n]}|}{\sqrt{1 - \alpha_n \bar{\alpha}_n}} \tag{2.5.5}$$

$$e^{2i(\theta_{n+1} - \theta_n)} = \frac{1 - \bar{\alpha}_n e^{-i[(n+1)\eta + 2\theta_n]}}{1 - \alpha_n e^{i[(n+1)\eta + 2\theta_n]}} \tag{2.5.6}$$

In essence, we have traded the Szegő recursion relation for a system of two first order recursion relations (2.5.5), (2.5.6). The usefulness of this system comes partly from the fact that (2.5.6) is a decoupled relation with no dependence on r_n. Note also that if $\alpha_n = 0$, (2.5.4) implies $\theta_{n+1} = \theta_n$. This justifies the addition of the $e^{in\eta}$ in (2.5.3) because we will use Prüfer variables to analyze perturbations around the free case $\alpha_n \equiv 0$, and now we can hope that if α_n is "small," then θ_n varies slowly in some sense.

The following lemma provides a criterion for the measure μ to have purely a.c. spectrum on an interval. This will be the basic criterion we will use in Chapter 4. Part (iii) of the lemma will be crucial for a proof by contradiction in Chapter 4.

Lemma 2.5.3. *Let a measure* $d\mu = w(e^{i\eta})\frac{d\eta}{2\pi} + d\mu_{\mathrm{s}}$ *on the unit circle have Verblunsky parameters* $\{\alpha_n\}_{n=0}^{\infty}$ *and Prüfer variables* $r_n(e^{i\eta})$.

(i) If $\log r_n(e^{i\eta})$ *converges uniformly on interval* $I \subset \partial\mathbb{D}$*, then*

$$\chi_I(e^{i\eta})d\mu(e^{i\eta}) = \chi_I(e^{i\eta})\frac{1}{\lim\limits_{n\to\infty} r_n^2(e^{i\eta})}\frac{d\eta}{2\pi} \tag{2.5.7}$$

so the measure μ *is purely absolutely continuous on* I *and* $w(e^{i\eta})$ *is continuous and strictly positive on* I*.*

(ii) If $S \subset \partial\mathbb{D}$ *is finite and* $\log r_n(e^{i\eta})$ *converges uniformly on intervals* $I \subset \partial\mathbb{D}$ *with* $\operatorname{dist}(I, S) > 0$*, then* $\operatorname{supp}\mu_{\mathrm{s}} \subset S$ *and* $w(e^{i\eta})$ *is continuous and strictly positive on* $\partial\mathbb{D} \setminus S$*.*

(iii) If $\alpha_n \to 0$*, it is not possible for* $\log r_n(e^{i\eta})$ *to converge as* $n \to \infty$ *to* $+\infty$ *or* $-\infty$ *uniformly on an interval* I*.*

Proof. (i) Note that $r_n(e^{i\eta}) = |\varphi_n(e^{i\eta})|$, so this is an immediate corollary of the Bernstein–Szegő approximations (Theorem 2.5.2).

(ii) Since S is finite, $\partial\mathbb{D} \setminus S$ can be covered by countably many intervals I with $\operatorname{dist}(I, S) > 0$. Applying (i) to each of them proves (ii).

(iii) If $r_n(e^{i\eta})$ converged uniformly to 0 or to $+\infty$ on I, Bernstein–Szegő approximations integrated against $\chi_I(e^{i\eta})$ would imply that $\mu(I) = \infty$ or $\mu(I) = 0$, contradicting either the assumption that $d\mu$ is a probability measure or Theorem 2.3.3. □

We will now see an application of Prüfer's variables. The following result is due to Baxter [1].

Theorem 2.5.4 (Baxter)**.** *If* $\{\alpha_n\} \in \ell^1$*, then the corresponding measure is purely absolutely continuous,* $d\mu = w(e^{i\theta})\frac{d\theta}{2\pi}$*, and* w *is continuous and strictly positive on* $\partial\mathbb{D}$*.*

Proof. Taking the real part of the logarithm of (2.5.4), we see

$$\log\frac{r_{n+1}(e^{i\eta})}{r_n(e^{i\eta})} = \operatorname{Re}\log(1 - \bar{\alpha}_n e^{-i[(n+1)\eta + 2\theta_n]}) - \tfrac{1}{2}\log(1 - |\alpha_n|^2) = O(|\alpha_n|)$$

Since $\alpha_n \to 0$, there exists a constant C independent of n or η such that

$$|\log r_{n+1}(e^{i\eta}) - \log r_n(e^{i\eta})| \le C|\alpha_n| \tag{2.5.8}$$

With $\{\alpha_n\} \in \ell^1$ and $\log r_0(e^{i\eta}) = 0$, (2.5.8) shows that the sequence $\log r_n(e^{i\eta})$ converges uniformly on $\partial\mathbb{D}$, so all the conclusions follow from Lemma 2.5.3(i). □

Baxter [1] actually proved a lot more, providing a necessary and sufficient condition for $\alpha \in \ell^1$ in terms of the moments of μ and other related results. For more information and contributions by Simon, including a criterion for w to be k times differentiable, see [60, Chapter 5].

We now proceed to the second criterion for a.c. spectrum. For this criterion, we will be interested in arbitrary solutions $\Psi_n(z) = \binom{\psi_n(z)}{\psi_n^*(z)}$ of the matrix recursion relation

$$\Psi_{n+1}(z) = A(\alpha_n, z)\Psi_n(z) \tag{2.5.9}$$

where

$$A(\alpha, z) = \frac{1}{\sqrt{1-|\alpha|^2}} \begin{pmatrix} z & -\bar{\alpha} \\ -\alpha z & 1 \end{pmatrix}$$

Note that ψ_n and ψ_n^* are not required to be related by any formula of the type (2.3.1) and should be seen as two a priori independent components of $\Psi_n(z)$. We will also denote $\Phi_n(z) = \binom{\varphi_n(z)}{\varphi_n^*(z)}$ and point out that $\Phi_n(z)$ is the solution with $\Phi_0(z) = \binom{1}{1}$.

Definition 2.5.1. For $z \in \partial\mathbb{D}$, $\{\Psi_n(z)\}_{n=0}^\infty$ is a *subordinate solution* at z if and only if for any solution $X_n(z)$ linearly independent with $\Psi_n(z)$,

$$\lim_{n\to\infty} \frac{\sum_{k=0}^n |\Psi_k(z)|^2}{\sum_{k=0}^n |X_k(z)|^2} = 0 \tag{2.5.10}$$

We also define

$$N = \{z \in \partial\mathbb{D} \mid \text{there is no subordinate solution at } z\} \tag{2.5.11}$$

and

$$S_1 = \{z \in \partial\mathbb{D} \mid \Phi_n(z) \text{ is a subordinate solution at } z\} \tag{2.5.12}$$

The extension of subordinacy theory to OPUC is due to Simon [60, Section 10.9]. We will state the relevant theorem without proof.

Theorem 2.5.5. *Let $d\mu(e^{i\theta}) = w(e^{i\theta})\frac{d\theta}{2\pi} + d\mu_{\mathrm{s}}$ and N and S_1 the corresponding sets defined in* (2.5.11), (2.5.12). *Up to a set of zero Lebesgue measure, the absolutely continuous part of μ is supported on N, i.e.*

$$m(N \triangle \{\theta \mid w(e^{i\theta}) \neq 0\}) = 0$$

Further, the singular part of μ_{s} is supported in S_1, $\operatorname{supp}\mu_{\mathrm{s}} \subset S_1$.

Chapter 3

Schrödinger operators

3.1 Introduction

In this chapter, we will introduce Schrödinger operators. In a narrow and informal sense, these are operators given by a formal expression

$$-\Delta + V(x) \tag{3.1.1}$$

acting on functions in $L^2(\Omega)$, where Ω is a region in $\mathbb{R}^d$, Δ stands for the Laplacian and $V(x)$ for pointwise multiplication by a real-valued function $V\colon \Omega \to \mathbb{R}$. Their name, and a part of the motivation for their study, comes from quantum mechanics, in which they determine the time-evolution of a particle confined to a region Ω, moving in the external potential V.

In the introduction to Chapter 1, we pointed out several subtleties involved with defining the Laplacian as an operator on $L^2(\mathbb{R}^n)$, and used them as motivation for our treatment of unbounded operators. We will now make a full circle and use the framework presented in Chapter 1 to discuss operators of the form (3.1.1).

In the examples in Section 1.5, we saw that questions of self-adjointness and spectrum of a differential operator depend greatly on the domain and choices of boundary conditions. It is thus not surprising that the one-dimensional case is much simpler than the general n-dimensional case, as there are, in a sense, only two boundary points to worry about. We will therefore begin our treatment with the one-dimensional case.

3.2 One-dimensional Schrödinger operators

In this section we will make sense of the formal expression $-\frac{d^2}{dx^2} + V$ as a differential operator on $L^2(I)$, where I is an interval, and we will see how choices of domain affect self-adjointness of H.

Let us start with an open interval $I = (a, b) \subset \mathbb{R}$ (a may be $-\infty$; b may be $+\infty$) and a real-valued function $V \in L^1_{\mathrm{loc}}(I)$. We want to define the formal expression

$$H = -\frac{d^2}{dx^2} + V$$

on functions f which have a sufficiently well-behaved weak first and second derivative that, for example, integration by parts still holds. We thus restrict to elements of

$$\mathrm{AC}^2_{\mathrm{loc}}(I) = \{f \in \mathrm{AC}_{\mathrm{loc}}(I) \mid f' \in \mathrm{AC}_{\mathrm{loc}}(I)\} \tag{3.2.1}$$

The choice to restrict to $\mathrm{AC}^2_{\mathrm{loc}}(I)$ is further backed by the following theorem, a standard result on existence and uniqueness of solutions of differential equations.

Theorem 3.2.1. *Let $x_0 \in I$ and $z, \alpha, \beta \in \mathbb{C}$. If $g \in L^1_{\mathrm{loc}}(I)$, then there exists a unique $f \in \mathrm{AC}^2_{\mathrm{loc}}(I)$ which is a solution of*

$$-f'' + (V - z)f = g \tag{3.2.2}$$

and has initial conditions

$$f(x_0) = \alpha, \quad f'(x_0) = \beta \tag{3.2.3}$$

Moreover, if V and g are L^1 in a neighborhood of a finite endpoint, then f and f' have finite limits at that endpoint.

Thus, by varying $\alpha, \beta \in \mathbb{C}$, we see the set of solutions to (3.2.2) is a two-dimensional vector space.

Proof. It is a standard trick (and it is straightforward to check) that the differential equation (3.2.2) together with initial conditions (3.2.3) is equivalent to an integral equation in terms of

$$F(x) = \begin{pmatrix} f(x) \\ f'(x) \end{pmatrix}, \quad G(x) = \begin{pmatrix} \alpha \\ \beta + \int_{x_0}^{x} g(y)dy \end{pmatrix}, \quad \tilde{V}(y) = \begin{pmatrix} 0 & 1 \\ V(y) - z & 0 \end{pmatrix}$$

known as the Volterra integral equation,

$$F(x) = G(x) + \int_{x_0}^{x} \tilde{V}(y)F(y)dy \tag{3.2.4}$$

so it suffices to prove that this integral equation has a unique solution. Fixing a compact interval $[c, d] \subset I$, we define the operator A on the space of continuous functions from $[c, d]$ to $\mathbb{C}^2$,

$$(AF)(x) = \int_{x_0}^{x} \tilde{V}(y)F(y)dy$$

and a simple induction argument establishes

$$(A^n F)(x) \leq \frac{\|F\|}{n!} \left| \int_{x_0}^{x} \|\tilde{V}(y)\| dy \right|^n \tag{3.2.5}$$

(here we are using $\|\tilde{V}\| \in L^1[c,d]$, which follows from $V \in L^1_{\text{loc}}$). With (3.2.5), iterating (3.2.4) implies that

$$F = \sum_{n=0}^{\infty} A^n G \tag{3.2.6}$$

Conversely, (3.2.6) defines a continuous function F on $[c,d]$ by (3.2.5), and by a direct substitution, this F solves (3.2.4). If a is a finite endpoint and V and g are L^1 up to the endpoint, the same proof goes through with $c = a$ and produces a solution F continuous at a. $\square$

Moreover, since H is to be an operator on $L^2(I)$, we take the domain of H to be

$$D(H) = \{f \in L^2(I) \mid f \in \mathrm{AC}^2_{\text{loc}}(I), -f'' + Vf \in L^2(I)\} \tag{3.2.7}$$

To determine the adjoint of H, using considerations similar to those in Example 1.5.2, one concludes that H is densely defined, $D(H^*) \subset D(H)$ and $H^* f = Hf$ for $f \in D(H^*)$. For $f, g \in D(H)$ and $a < c < d < b$, a double integration by parts gives

$$\int_c^d (\bar{g}Hf - \overline{Hg}f)dx = W_d(\bar{g}, f) - W_c(\bar{g}, f) \tag{3.2.8}$$

where for $x \in I$, the Wronskian $W_x(\bar{g}, f)$ is given by

$$W_x(\bar{g}, f) = \overline{g(x)} f'(x) - \overline{g'(x)} f(x) \tag{3.2.9}$$

Since $f, g, Hf, Hg \in L^2(I)$, Cauchy–Schwarz implies that $\bar{g}Hf, \overline{Hg}f \in L^1(I)$. Thus, dominated convergence implies that (3.2.8) has finite limits as $c \downarrow a$ or $d \uparrow b$, so the Wronskian (3.2.9) has limits as $x \downarrow a$ or $x \uparrow b$. We will usually denote these limits simply by $W_a(\bar{g}, f)$, $W_b(\bar{g}, f)$.

Taking the limit of (3.2.8) as $c \downarrow a$ and $d \uparrow b$, we now have

$$\langle g, Hf \rangle - \langle Hg, f \rangle = W_b(\bar{g}, f) - W_a(\bar{g}, f) \tag{3.2.10}$$

Remember that $g \in D(H^*)$ if and only if the left-hand side of (3.2.10) is equal to 0 for all $f \in D(H)$, so we can now describe $D(H^*)$:

$$D(H^*) = \{g \in D(H) \mid W_b(\bar{g}, f) - W_a(\bar{g}, f) = 0 \quad \forall f \in D(H)\} \tag{3.2.11}$$

In some situations we may prefer to restate this in a different form. Note that for any $f \in D(H)$, one can find $h \in D(H)$ such that $h(x) = f(x)$ in a neighborhood of a and $h(x) = 0$ in a neighborhood of b. Applying (3.2.10) with h and $f - h$ instead of f, we see that

$$D(H^*) = \{g \in D(H) \mid W_a(\bar{g}, f) = W_b(\bar{g}, f) = 0 \quad \forall f \in D(H)\} \tag{3.2.12}$$

In the next section, we will continue this analysis, with the goal of describing all self-adjoint restrictions of H.

3.3 The limit point–limit circle alternative

Naive considerations might lead one to think that each of the conditions $W_a(\bar{g}, f) = 0$ and $W_b(\bar{g}, f) = 0$ restricts the set of g by setting conditions on behavior of g and g' near a, so that $D(H^*)$ has (complex) codimension 4 in $D(H)$. It is in fact obvious that the codimension is at most 4, since by the discussion of deficiency indices in Section 1.3 and by Theorem 3.2.1, the codimension is $\dim \operatorname{Ker}(H - i) + \dim \operatorname{Ker}(H + i) \leq 4$. Further, complex conjugation is an isomorphism between $\operatorname{Ker}(H - i)$ and $\operatorname{Ker}(H + i)$, so

$$\dim \operatorname{Ker}(H - i) + \dim \operatorname{Ker}(H + i) \in \{0, 2, 4\}$$

However, one or both of the Wronskian conditions may be satisfied identically so the codimension may be less than 4, and in particular, $D(H^*)$ may even be equal to $D(H)$. A celebrated result of Weyl [79] describes this dichotomy and uses it to describe self-adjoint restrictions of H.

Definition 3.3.1. The operator H is *limit point* at an endpoint $c \in \{a, b\}$ if and only if

$$W_c(f, g) = 0, \quad \forall f, g \in D(H) \tag{3.3.1}$$

Otherwise, it is *limit circle* at c.

Note that (3.3.1) is a local condition around the endpoint, so this property depends only on the behavior of V in a neighborhood of the endpoint. However, we are about to relate it to self-adjointness of H.

The following bilinear form will be important:

$$S(u, v) = W_b(u, v) - W_a(u, v) \tag{3.3.2}$$

Theorem 3.3.1. *(i) If H is limit point at both a and b, then H is self-adjoint.*

(ii) If H is limit point at exactly one endpoint, then all the self-adjoint restrictions of H are

described by

$$D(H_v) = \{f \in D(H) \mid S(\bar{v}, f) = 0\} \tag{3.3.3}$$

for some $v \in D(H) \setminus D(H^*)$ *such that* $S(\bar{v}, v) = 0$.

(iii) If H *is limit circle at both endpoints, all the self-adjoint restrictions of* H *are described by*

$$D(H_{u,v}) = \{f \in D(H) \mid S(\bar{u}, f) = S(\bar{v}, f) = 0\} \tag{3.3.4}$$

with $u, v \in D(H) \setminus D(H^*)$ *such that* $S(\bar{u}, u) = S(\bar{u}, v) = S(\bar{v}, v) = 0$.

We see that if a is limit circle, the key are $v \in D(H) \setminus D(H^*)$ such that $W_a(\bar{v}, v) = 0$. To see that such v exist, first let v be such that $W_a(v, \cdot)$ is not identically 0. Then the same holds for $\operatorname{Re} v$ or $\operatorname{Im} v$, so we can pick v to be real-valued. However, for v real-valued, $W_a(\bar{v}, v) = 0$ is trivial.

Before we proceed to the proof, we will prove a simple lemma.

Lemma 3.3.2. *(i) (Plücker identity) For all* $u_1, u_2, u_3, u_4 \in D(H)$, *we have*

$$W_x(u_1, u_2)W_x(u_3, u_4) - W_x(u_1, u_3)W_x(u_2, u_4) + W_x(u_1, u_4)W_x(u_2, u_3) = 0$$

(ii) Let $u, v \in D(H)$ *be such that* $W_a(u, v) \neq 0$. *Then for any* $f, g \in D(H)$,

$$W_a(u, f) = W_a(v, f) = 0 \implies W_a(g, f) = 0$$

Proof. (i) For $x \in I$, this follows from the obvious

$$\begin{vmatrix} u_1(x) & u_2(x) & u_3(x) & u_4(x) \\ u_1'(x) & u_2'(x) & u_3'(x) & u_4'(x) \\ u_1(x) & u_2(x) & u_3(x) & u_4(x) \\ u_1'(x) & u_2'(x) & u_3'(x) & u_4'(x) \end{vmatrix} = 0$$

and for $x \in \{a, b\}$, it follows by taking the limit as $x \downarrow a$ or $x \uparrow b$.

(ii) This is an immediate corollary of (i) applied to u, v, f, g. □

Proof of Theorem 3.3.1. We denote $X = D(H)/D(H^*)$ and we denote its elements by $[u] = u + D(H^*)$. Note that $X = X_a \oplus X_b$, where

$$X_a = \{[u] \mid W_b(u, f) = 0 \quad \forall f \in D(H)\}$$

$$X_b = \{[u] \mid W_a(u, f) = 0 \quad \forall f \in D(H)\}$$

Clearly, if H is limit point at a, then $\dim X_a = 0$. If H is limit circle at a, we will show that $\dim X_a = 2$. Since H is limit circle at a, there exist $u, v \in D(H)$ with $W_a(u,v) \neq 0$. Since $W_a(u,u) = 0$, $[u]$ and $[v]$ are linearly independent in X_a, so $\dim X_a \geq 2$. For any $h \in X_a$, $h = \alpha u + \beta v + f$ with $W_a(f,u) = W_a(f,v) = 0$, but then Lemma 3.3.2(ii) implies $[f] = 0$. Thus, $\dim X_a = 2$.

Analogous arguments apply to the endpoint b, so we conclude

$$\dim X = \begin{cases} 0, & \text{if } H \text{ is limit point at both endpoints} \\ 2, & \text{if } H \text{ is limit circle at exactly one endpoint} \\ 4, & \text{if } H \text{ is limit circle at both endpoints} \end{cases}$$

By (3.2.11), a bilinear form $\tilde{S}\colon X \times X \to \mathbb{C}$ is induced by (3.3.2),

$$\tilde{S}([u],[v]) = S(u,v)$$

Note that by (3.2.11), for $[u] \neq 0$, $\tilde{S}([u],\cdot)$ is not identically 0, so $\tilde{S}$ is a nondegenerate bilinear form. We remind the reader that for such $\tilde{S}$, one can define orthogonality in the same way, and with much the same properties, as one would if $\tilde{S}$ was an inner product.

Any operator $\tilde{H}$ with $\Gamma(H^*) \subset \Gamma(\tilde{H}) \subset \Gamma(H)$ is uniquely determined by its domain $D(\tilde{H})$, so by a vector subspace $U = D(\tilde{H})/D(H^*) \subset X$. Note that its adjoint $\tilde{H}^*$ also has $\Gamma(H^*) \subset \Gamma(\tilde{H}^*) \subset \Gamma(H)$, so corresponds to $U^* = D(\tilde{H}^*)/D(H^*) \subset X$. By (3.2.10),

$$U^* = \{\bar{u} \mid u \in U^\perp\}$$

with orthogonality provided by the sesquilinear form $\tilde{S}$. Clearly, $\tilde{H}$ will be self-adjoint if and only if $U = U^*$. Thus, self-adjoint extensions of H are in 1-1 correspondence with subspaces U of X such that $\dim U = \dim X/2$ and

$$\tilde{S}([\bar{u}],[v]) = 0, \quad \forall [u],[v] \in U$$

Specializing this to the cases $\dim X = 0, 2, 4$ provides parts (i)–(iii) of the theorem. $\square$

In the remainder of this section, we will present some criteria that can be used to determine whether H is in the limit point or in the limit circle case at its endpoints. We start by introducing regular endpoints.

Definition 3.3.2. We say that a is a *regular endpoint* of H if a is a finite endpoint ($a \neq -\infty$) and $V \in L^1(a,c)$ for some $c \in I$, and a *singular endpoint* otherwise, and similarly for b.

Informally speaking, regular endpoints are significant because they behave very much like interior points of I. The following result will be a corollary of Theorem 3.2.1.

Theorem 3.3.3. *Let a be a regular endpoint of H. Then for every $f \in D(H)$, f and f' can be continuously extended to $\{a\} \cup I$ and are absolutely continuous on $[a, d]$ for $d \in I$. Thus, existence and uniqueness of solutions of* (3.2.2) *with initial conditions* (3.2.3) *holds for $x_0 = a$. In particular, H is limit circle at a.*

Proof. Since $f \in D(H)$, we have $g = -f'' + Vf \in L^2(I)$, so $g \in L^2(a, a+\epsilon) \subset L^1(a, a+\epsilon)$. Thus, continuity of f, f' at a follows from Theorem 3.2.1, and the proof of Theorem 3.2.1 is valid for $x_0 = a$. Finally, note that since we can prescribe values of f, f' at a arbitrarily, there exist $f, g \in D(H)$ with $f(a) = 1$, $f'(a) = 0$, $g(a) = 0$, $g'(a) = 1$, so $W_a(f, g) = 1$, proving that H is limit circle at a. □

Example 3.3.1. Let $I = (0, +\infty)$ and $V \equiv 0$. The operator $H = -\frac{d^2}{dx^2}$ is limit circle at 0 and limit point at ∞, and self-adjoint restrictions of H are parametrized by $\theta \in [0, \pi)$ so that

$$D(H_\theta) = \{f \in D(H) \mid \cos\theta f(0) + \sin\theta f'(0) = 0\} \tag{3.3.5}$$

Proof. By Theorem 3.3.3, H is limit circle at 0. To see that it is limit point at ∞, solve the equation $-f'' - if = 0$. Two linearly independent solutions are

$$f_\pm(x) = \exp(\pm e^{-i\pi/4} x)$$

Since $f_+ \in L^2(0, \infty)$ but $f_- \notin L^2(0, \infty)$, we see that $\dim \operatorname{Ker}(H - i) = 1$, so by theorem 3.3.1, H is limit point at ∞.

An arbitrary self-adjoint restriction corresponds to a choice of $v \in D(H)$ with $W_0(\bar{v}, v) = 0$ and $W_0(v, \cdot)$ not identically 0.

By Theorem 3.3.3, for any $v, f \in D(H)$,

$$W_0(v, f) = v(0)f'(0) - v'(0)f(0)$$

so we see $W_0(v, \cdot)$ is identically 0 if and only if $v(0) = v'(0) = 0$, and $W_0(\bar{v}, v) = 0$ if and only if $\overline{v(0)}v'(0) \in \mathbb{R}$. By factoring out an irrelevant multiplicative constant from v, we can bring it to the form $v(0), v'(0) \in \mathbb{R}$, $v(0) + iv'(0) = e^{-i\theta}$, $\theta \in [0, \pi)$, which gives (3.3.5). □

Theorem 3.3.3 provides a sufficient condition for a Schrödinger operator to be limit circle at a finite endpoint, but the condition is very strong. We will now present without proof some other sufficient conditions for H to be limit point or limit circle at an endpoint. The conditions are different for finite endpoints than for infinite endpoints, and since our later focus will be on Schrödinger operators on a half-line $I = (0, +\infty)$, we will present the criteria for 0 and $+\infty$. The reader can easily formulate the general case by translation and reflection of the real line.

Theorem 3.3.4 (Kostenko–Sakhnovich–Teschl [39]). *Let $H = -\Delta + V$ be a Schrödinger operator on $(0, 1)$. Assume that for some $l \geq -\frac{1}{2}$,*

$$V(x) = \frac{l(l+1)}{x^2} + q(x)$$

with q real-valued such that

$$xq(x) \in L^1(0,1), \text{ if } l > -\tfrac{1}{2}$$
$$x(1 - \log(x))q(x) \in L^1(0,1), \text{ if } l = -\tfrac{1}{2}$$

Then H is limit point at 0 if and only if $l \geq \frac{1}{2}$. For $l \in [-\frac{1}{2}, \frac{1}{2})$, one possible choice of self-adjoint boundary condition is

$$\lim_{x \downarrow 0} x^l((l+1)f(x) - xf'(x)) = 0 \tag{3.3.6}$$

If $\tilde{H}$ is the restriction of H obtained by imposing the boundary condition (3.3.6) *(if needed), the spectrum of $\tilde{H}$ is purely discrete and bounded from below.*

Theorem 3.3.5. *Let $V \in L^1_{\text{loc}}(0, +\infty)$ and*

$$\limsup_{n\to\infty} \int_n^{n+1} |V(x)| dx < \infty$$

Then H is limit point at $+\infty$.

Finally, we will need a result on preservation of essential spectrum.

Theorem 3.3.6. *Let $V \in L^1_{\text{loc}}(0, +\infty)$ and*

$$\lim_{n\to\infty} \int_n^{n+1} |V(x)| dx = 0 \tag{3.3.7}$$

Assume further that $H = -\Delta + V$ is regular at 0. Then $\sigma_{\text{ess}}(H) = [0, +\infty)$.

The proof relies on Weyl's theorem and comparison with the free Schrödinger operator H_0 given in Example 3.3.1. However, applying it directly to H and H_0 wouldn't work, so one uses resolvents and proves that $R_z(H) - R_z(H_0)$ is compact when (3.3.7) holds. For details, see [72, Section 9.7].

3.4 Locating the a.c. spectrum

In this section we will present the subordinacy theory of Gilbert–Pearson [25], which describes the a.c. spectrum in terms of the asymptotics of formal solutions of $-u'' + Vu = Eu$. We will also define Prüfer variables, which will be a very convenient tool in controlling the asymptotics of formal solutions.

As a first result, we present subordinacy theory for a Schrödinger operator with a regular endpoint.

Definition 3.4.1. Let H be regular at a. A solution of $-u'' + Vu = Eu$ is *subordinate* if for any linearly independent solution v of the same equation,

$$\lim_{x \uparrow b} \frac{\int_a^x |u(y)|^2 dy}{\int_a^x |v(y)|^2 dy} = 0$$

Theorem 3.4.1 (Gilbert–Pearson)**.** *Let H_θ be regular at a with boundary condition*

$$\cos\theta f(a) + \sin\theta f'(a) = 0 \tag{3.4.1}$$

Let N be the set of $E \in \mathbb{R}$ for which there is no subordinate solution and let S be the set of $E \in \mathbb{R}$ for which there exists a subordinate solution u which satisfies the boundary condition (3.4.1)*. The set N is a minimal support for the a.c. spectrum of H_θ, i.e.*

$$\sigma_{\mathrm{ac}}(H_\theta) = \overline{N}^{\mathrm{ess}}$$

and the set S is a support for the singular spectrum of H_θ.

The next example revisits the self-adjoint realizations H_θ of the free Laplacian on a half-line, introduced in Example 3.3.1.

Example 3.4.1. Using the notation from Example 3.3.1, H_θ has

$$\sigma_{\mathrm{ac}}(H_\theta) = [0, +\infty) \tag{3.4.2}$$

$$\sigma_{\mathrm{sc}}(H_\theta) = \emptyset \tag{3.4.3}$$

$$\sigma_{\mathrm{pp}}(H) = \begin{cases} \{-\cot^2\theta\}, & \theta \in (0, \pi/2) \\ \emptyset, & \theta \in \{0\} \cup [\pi/2, \pi) \end{cases} \tag{3.4.4}$$

Proof. For $E > 0$, $-u'' = Eu$ has solutions $u = C\cos(\sqrt{E}\,x + \phi)$, so it is straightforward to see that there are no subordinate solutions. Thus, $(0, \infty) \subset N$.

For $E = 0$, $-u'' = 0$ has solutions $u = A + Bx$, so $u = 1$ is a subordinate solution, which satisfies the boundary condition (3.4.1) for $\theta = 0$. For $E < 0$, $-u'' = Eu$ has solutions

$$u = A\exp(\sqrt{-E}\,x) + B\exp(-\sqrt{-E}\,x)$$

so a subordinate solution is $u = \exp(-\sqrt{-E}\,x)$. It satisfies the boundary condition (3.4.1) when $\sqrt{-E} = \cot\theta$; note that this implies $\cot\theta > 0$, so $\theta \in (0, \pi/2)$.

Thus, for any θ, $N = (0, \infty)$, which implies (3.4.2) by Theorem 3.4.1. To conclude (3.4.3) and (3.4.4), note that by Theorem 3.4.1 and the previous considerations,

$$\sigma_{\text{sing}}(H_\theta) = \begin{cases} \{0\}, & \theta = 0 \\ \{-\cot^2\theta\}, & \theta \in (0, \pi/2) \\ \emptyset, & \theta \in [\pi/2, \pi) \end{cases}$$

Since a single-element set cannot support continuous spectrum, this immediately implies (3.4.3). Note that $u \equiv 1$ is not an element of $L^2(0, \infty)$, so it is not an eigenvalue of H_0 and $\sigma_{\text{pp}}(H_0) = \emptyset$. For $\theta \in (0, \pi/2)$, $u = \exp(-\cot\theta\, x)$ is indeed an eigenvalue of H_θ, so the proof of (3.4.4) is complete. □

The next result will abandon the restriction that one of the endpoints must be regular. Then one may pick $c \in (a, b)$ and define subordinate solutions as above, but with integration from c:

Definition 3.4.2. A nontrivial solution of $-u'' + Vu = Eu$ is *subordinate at a* if for any linearly independent solution v of the same equation,

$$\lim_{x \downarrow a} \frac{\int_x^c |u(y)|^2 dy}{\int_x^c |v(y)|^2 dy} = 0 \tag{3.4.5}$$

Analogously, it is subordinate at b if for any linearly independent solution v of the same equation,

$$\lim_{x \uparrow b} \frac{\int_c^x |u(y)|^2 dy}{\int_c^x |v(y)|^2 dy} = 0 \tag{3.4.6}$$

Theorem 3.4.2. *For an endpoint $c \in \{a, b\}$, denote by N_c the set of $E \in \mathbb{R}$ for which there is no subordinate solution at c. Denote by S the set of $E \in \mathbb{R}$ for which there exists a solution which is subordinate at both a and b. Then*

$$\sigma_{\text{ac}}(H) = (\overline{N_a \cup N_b})^{\text{ess}}$$

and the singular spectrum of H is supported in S.

As our last topic in this section, we define Prüfer variables. From now on, we will work on the half-line $I = (0, +\infty)$. Because we do not assume 0 is a regular point, we will set all our initial conditions at an arbitrary $c \in I$. For $E = \eta^2/4$ with $\eta > 0$ and a real-valued solution $u(x)$ of

$$Hu = Eu \tag{3.4.7}$$

we define modified Prüfer variables by

$$u'(x) = \tfrac{1}{2}\eta R_\eta(x)\cos(\tfrac{1}{2}\eta x + \theta_\eta(x)) \tag{3.4.8}$$

$$u(x) = R_\eta(x)\sin(\tfrac{1}{2}\eta x + \theta_\eta(x)) \tag{3.4.9}$$

The 2π ambiguity in $\theta_\eta(x)$ is partly fixed by making $\theta_\eta(x)$ continuous in x; there is still a 2π ambiguity in $\theta_\eta(c)$, and any choice will be equally good for our analysis. Substituting into (3.4.7), we obtain a system of first-order differential equations for $\log R_\eta$ and θ_η,

$$\frac{d\theta_\eta}{dx} = -2\frac{V(x)}{\eta}\sin^2(\tfrac{1}{2}\eta x + \theta_\eta(x)) \tag{3.4.10}$$

$$\frac{d}{dx}\log R_\eta(x) = \frac{V(x)}{\eta}\sin(\eta x + 2\theta_\eta(x)) \tag{3.4.11}$$

with initial values $R_\eta(c) > 0$, $\theta_\eta(c) \in \mathbb{R}$. We have departed from the usual notation by parametrizing in $\eta = 2\sqrt{E}$ rather than $k = \sqrt{E}$. This will later make our notation more consistent with that used for orthogonal polynomials. We have also made a non-standard modification to include $\frac{1}{2}\eta x$ in (3.4.8), (3.4.9). With this change, if $V = 0$ in some interval, then θ_η is constant in that interval by (3.4.10).

It will be convenient to rewrite (3.4.10) and (3.4.11) in terms of complex exponentials, as

$$\frac{d\theta_\eta}{dx} = -\frac{V(x)}{\eta}\big(1 - e^{i[\eta x + 2\theta_\eta(x)]} - e^{-i[\eta x + 2\theta_\eta(x)]}\big) \tag{3.4.12}$$

$$\frac{d}{dx}\log R_\eta(x) = \operatorname{Im}\Big(\frac{V(x)}{\eta}e^{i[\eta x + 2\theta_\eta(x)]}\Big) \tag{3.4.13}$$

The following simple lemma shows how Prüfer variables can be used to prove nonexistence of subordinate solutions.

Lemma 3.4.3. *Assume that*

$$\sup_x \int_x^{x+1} |V(y)|dy < \infty \tag{3.4.14}$$

If for $E = \eta^2/4$ *in some set* S, $R_\eta(x)$ *is bounded as* $x \to \infty$ *for any initial conditions* $R_\eta(c)$, $\theta_\eta(c)$, *then* H *has purely absolutely continuous spectrum on* S *and the spectral measure is mutually absolutely continuous on* S *with the Lebesgue measure.*

Boundedness of $R_\eta(x)$ implies boundedness of all complex solutions of $Hu = Eu$, and it is an observation of Behncke [2] and Stolz [65] that (3.4.14) and boundedness of eigenfunctions allows one to use subordinacy theory to imply the conclusions of the lemma. A different proof is due to Simon [59].

Theorem 3.4.4. *If* $V \in L^1(0,\infty)$, *then* $\sigma_{\rm ac}(H) = [0,+\infty)$, $\sigma_{\rm sc}(H) = \emptyset$ *and* $\sigma_{\rm pp}(H) \subset (-\infty, 0]$.

Proof. For $\eta > 0$, (3.4.13) implies

$$\Big|\frac{d}{dx}\log R_\eta(x)\Big| \le \frac{1}{\eta}|V(x)|$$

so $V \in L^1(0,\infty)$ implies that $\log R_\eta(x)$ converges as $x \to \infty$, so by Lemma 3.4.3, $(0,+\infty) \subset N_\infty$. By Theorem 3.4.1, this implies $[0,+\infty) \subset \sigma_{\mathrm{ac}}(H)$ and $\sigma_{\mathrm{s}}(H) \subset (-\infty,0]$. However, note that dominated convergence with V as the dominating function implies that (3.3.7) holds, so by Theorem 3.3.6, $\sigma_{\mathrm{ess}} = [0,+\infty)$, which completes the proof. □

3.5 Spherically symmetric Schrödinger operators

As we have mentioned before, for Schrödinger operators in more than one dimension the question of self-adjointness and boundary conditions is much more subtle. We will focus on the case when $V(x)$ is a function of $|x|$ alone and quote a result from Reed–Simon [50, Appendix to Section X.1, Example 4]. This will be a decomposition theorem which, under certain conditions, reduces spherically symmetric Schrödinger operators to a direct sum of half-line Schrödinger operators.

For $j \in \mathbb{N}_0$, we denote $\mu_j = j(j+n-2)$,

$$\lambda_j = \begin{cases} \frac{2j+n-2}{j}\binom{j+n-3}{j-1}, & j \ge 1 \\ 1, & j = 0 \end{cases}$$

(the values of λ_j and μ_j are not computed in [50]; see Weidmann [77, p. 299] for the proof) and operators

$$H_j = -\Delta + \Big(\mu_j + \frac{(n-1)(n-3)}{4}\Big)\frac{1}{r^2} + V(r) \tag{3.5.1}$$

on $L^2(0,\infty)$. As we are about to see, we will only use (3.5.1) where they are limit point at both 0 and ∞, so there is no need to specify boundary conditions.

Theorem 3.5.1. *Let $V \in L^2_{\mathrm{loc}}(\mathbb{R}^n \setminus \{0\})$ be a radial potential, $V(x) = V(|x|)$. If*

$$V(r) + \frac{(n-1)(n-3)}{4}\frac{1}{r^2} \ge \frac{3}{4r^2}$$

then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \setminus \{0\})$, all the H_j given by (3.5.1) are essentially self-adjoint on $C_0^\infty(0,+\infty)$ and $H = -\Delta + V$ is unitarily equivalent to the direct sum of operators H_j, with H_j repeated λ_j times.

Chapter 4

Generalized bounded variation perturbations

4.1 History and motivation for the problem

In Chapters 2 and 3, we have introduced OPRL, OPUC, and Schrödinger operators on a half-line, three systems which will now be of interest. In each of the systems, a free case has been singled out ($a_n \equiv 1$, $b_n \equiv 0$ for OPRL; $\alpha_n \equiv 0$ for OPUC; $V \equiv 0$ for Schrödinger operators). We will now focus on objects which are, in some sense, close to the free case, and we will think of them as perturbations around the free case. We wish to know what properties of the spectrum are preserved under certain perturbations.

We have already seen some results of this kind. Theorems 2.2.3, 2.3.3 and 3.3.6 all tell us that with decay of the perturbation at ∞, the essential spectrum remains preserved. With a much stronger condition, we can conclude more: Theorems 2.4.3, 2.5.4 and 3.4.4 tell us that an L^1 condition on the perturbation implies preservation of purely a.c. spectrum in the interior of the essential spectrum. We will now discuss results which fall between these two.

It is well known that bounded variation combined with decay of the perturbation implies preservation of a.c. spectrum. Weidmann [77] proved the first result of this kind, for Schrödinger operators (and, more generally, for Sturm–Liouville operators).

Theorem 4.1.1 (Weidmann)**.** *Let V be a potential on $[0,\infty)$ which can be expressed as $V = V_1 + V_2$, where V_1 has bounded variation, $\lim_{x\to\infty} V_1(x) = 0$ and $V_2 \in L^1(0,\infty)$. The corresponding Schrödinger operator $H = -\Delta + V$ has $\sigma_{\rm ac}(H) = [0,\infty)$, $\sigma_{\rm sc}(H) = \emptyset$ and $\sigma_{\rm pp}(H) \subset (-\infty, 0]$.*

The analogous results for OPRL and OPUC are due to Máté–Nevai [42] and Peherstorfer–Steinbauer [47].

Theorem 4.1.2 (Máté–Nevai)**.** *Let a sequence $\{a_n, b_n\}_{n=1}^{\infty}$ of Jacobi coefficients be such that $a_n \to$*

1, $b_n \to 0$, and

$$\sum_{n=1}^{\infty}|a_{n+1}-a_n|+\sum_{n=1}^{\infty}|b_{n+1}-b_n|<\infty$$

The corresponding measure $d\rho = f dx + d\rho_{\mathrm{s}}$ is purely absolutely continuous on $(-2,2)$ and $f(x)$ is continuous and strictly positive on $(-2,2)$.

Theorem 4.1.3 (Peherstorfer–Steinbauer)**.** *If a sequence of Verblunsky coefficients $\{\alpha_n\}_{n=0}^{\infty}$ has bounded variation and $\lim_{n\to\infty}\alpha_n = 0$, then the corresponding measure $d\mu = w(e^{i\theta})\frac{d\theta}{2\pi} + d\mu_{\mathrm{s}}$ is purely absolutely continuous on $\partial\mathbb{D}\setminus\{1\}$ and $w(e^{i\theta})$ is continuous and strictly positive on $\partial\mathbb{D}\setminus\{1\}$.*

Rotating a measure on $\partial\mathbb{D}$ by an angle ϕ gives an immediate corollary of Theorem 4.1.3.

Corollary 4.1.4. *If a sequence of Verblunsky coefficients $\{\alpha_n\}_{n=0}^{\infty}$ obeys*

$$\sum_{n=0}^{\infty}|e^{i\phi}\alpha_{n+1}-\alpha_n|<\infty \tag{4.1.1}$$

and $\lim_{n\to\infty}\alpha_n = 0$, then the corresponding measure $d\mu = w(e^{i\theta})\frac{d\theta}{2\pi}+d\mu_{\mathrm{s}}$ is purely absolutely continuous on $\partial\mathbb{D}\setminus\{e^{i\phi}\}$ and $w(e^{i\theta})$ is continuous and strictly positive on $\partial\mathbb{D}\setminus\{e^{i\phi}\}$.

It is thus natural to think of (4.1.1) as a kind of rotated bounded variation condition and to wonder what happens if α_n is a linear combination of such sequences. We will give a name to this property, which will be central to our results.

Definition 4.1.1. A sequence $\beta = \{\beta_n\}_{n=N}^{\infty}$ (N can be finite or $-\infty$) has *rotated bounded variation* with phase ϕ if

$$\sum_{n=N}^{\infty}|e^{i\phi}\beta_{n+1}-\beta_n|<\infty \tag{4.1.2}$$

A sequence $\alpha = \{\alpha_n\}_{n=N}^{\infty}$ has *generalized bounded variation* with the set of phases $A = \{\phi_1,\dots,\phi_L\}$, $L<\infty$, if it can be expressed as a sum

$$\alpha_n = \sum_{l=1}^{L}\beta_n^{(l)} \tag{4.1.3}$$

such that the l-th sequence $\beta^{(l)}$ has rotated bounded variation with phase ϕ_l.

The set of sequences having generalized bounded variation with the set of phases A will be denoted $GBV(A)$ or, with a slight abuse of notation, $GBV(\phi_1,\dots,\phi_L)$. In particular, $GBV(\phi)$ is the set of sequences with rotated bounded variation with phase ϕ.

Our results will use this notion of generalized bounded variation as the central assumption. An OPUC result of Wong [80], which uses this assumption, was the primary motivation for our work.

Theorem 4.1.5 (Wong)**.** *Let* $\alpha = \{\alpha_n\}_{n=0}^\infty$ *be a sequence of Verblunsky coefficients corresponding to* $d\mu = w(e^{i\theta})\frac{d\theta}{2\pi} + d\mu_{\mathrm{s}}$*. Let* α *have generalized bounded variation with the set of phases* A*, and let* $\alpha \in \ell^2$*. The measure* μ *is then purely absolutely continuous on* $\partial\mathbb{D} \setminus \{e^{i\eta} \mid \eta \in A\}$ *and* $w(e^{i\theta})$ *is continuous and strictly positive on* $\partial\mathbb{D} \setminus \{e^{i\eta} \mid \eta \in A\}$*.*

The original paper [80] assumes $\beta^{(l)} \in \ell^2$ for all $\beta^{(l)}$ in the decomposition (4.1.3), instead of assuming $\alpha \in \ell^2$. However, this seemingly weaker condition is in fact equivalent to $\alpha \in \ell^2$ by Lemma 4.3.1 below. Our OPUC result will be a generalization of Theorem 4.1.5 which substitutes the ℓ^2 assumption by an ℓ^p assumption, for any $p < \infty$.

For an example of a sequence with rotated bounded variation with phase ϕ, take

$$\beta_n = e^{-i(n\phi+\alpha)} B_n$$

where $\{B_n\}_{n=N}^\infty$ is any sequence of bounded variation; the first example that comes to mind is $B_n = n^{-\gamma}$. Generalized bounded variation may seem like an unnatural condition for real-valued sequences, but by combining rotated bounded variation with phases ϕ and $-\phi$, one gets

$$\frac{e^{-i(n\phi+\alpha)}}{n^\gamma} + \frac{e^{+i(n\phi+\alpha)}}{n^\gamma} = \frac{\cos(n\phi+\alpha)}{n^\gamma}$$

Trivially, any ℓ^1 sequence has rotated bounded variation with any phase ϕ. It follows from these observations that a linear combination

$$V_n = \sum_{k=1}^K \lambda_k \frac{\cos(n\phi_k + \alpha_k)}{n^{\gamma_k}} + W_n, \quad \gamma_k > 0, \quad \{W_n\} \in \ell^1 \tag{4.1.4}$$

has generalized bounded variation with the set of phases $\{\pm\phi_1, \pm\phi_2, \dots, \pm\phi_K\}$.

Discrete Schrödinger operators with potentials of the form (4.1.4) have been studied; the ℓ^2 case follows from a result of Kiselev–Last–Simon [38, Theorem 3.3], and a recent result of Janas–Simonov [32] goes beyond ℓ^2:

Theorem 4.1.6 (Janas–Simonov)**.** *Let a measure* $d\rho = f\,dx + d\rho_{\mathrm{s}}$ *have Jacobi parameters* $a_n \equiv 1$ *and*

$$b_n = \lambda \frac{\cos(n\phi+\alpha)}{n^\gamma} + W_n$$

with $\gamma > \frac{1}{3}$ *and* $\{W_n\} \in \ell^1$*. The measure* $d\rho$ *is then purely absolutely continuous on* $(-2,2) \setminus \{\pm 2\cos\phi, \pm 2\cos(\phi/2)\}$ *with* f *continuous and strictly positive on that set.*

Potentials of the form (4.1.4) are known as Wigner–von Neumann potentials because of work of Wigner and von Neumann [76] in which they constructed a Schrödinger operator on $(0, +\infty)$ whose potential has the asymptotic behavior

$$V(x) = -8\frac{\sin(2x)}{x} + O(x^{-2}), \quad x \to \infty \tag{4.1.5}$$

with the peculiar property that the Schrödinger operator $-\Delta + V$ has an eigenvalue at $+1$ embedded in the a.c. spectrum $[0, +\infty)$. More information on this example can be found in [52, Section XIII.13].

In the Schrödinger operator literature, Wigner–von Neumann potentials

$$V(x) = \sum_{k=1}^{K} \lambda_k \frac{\cos(\phi_k x + \alpha_k)}{x^{\gamma_k}} + W(x), \quad \gamma_k > 0, \quad W(x) \in L^1 \tag{4.1.6}$$

have been the subject of much research. For example, Reed–Simon [51, Section XI.8] analyze (4.1.6) in the case $\gamma_k = 1$, $W(x) = O(x^{-1-\epsilon})$; Ben-Artzi–Devinatz [3] analyze (4.1.6) in the case $K = 1$, $\gamma_1 > \frac{1}{2}$, $W(x) = O(x^{-1-\epsilon})$, as well as the more general $V(x) = a\cos(\phi x^\alpha)/x^\gamma + W(x)$ in some range of α, γ. A result of Harris–Lutz [28] (with a different proof by Kiselev–Last–Simon [38, Theorem 3.2]) settles the spectral analysis in the L^2 case.

Theorem 4.1.7 (Harris–Lutz)**.** *If V is of the form* (4.1.6) *with $\gamma_k > \frac{1}{2}$, then the spectral measure of $H = -\Delta + V$ is purely absolutely continuous on*

$$(0, \infty) \setminus \left\{ \frac{\phi_k^2}{4} \,\middle|\, 1 \le k \le K \right\}$$

We now define the notion of generalized bounded variation condition for functions. This notion is very much analogous to the condition for sequences, but with one difference: any ℓ^1 sequence has bounded variation, but L^1 functions do not necessarily have bounded variation. Since we want to allow presence of an L^1 term, we adjust the definition to explicitly allow it.

Definition 4.1.2. A function $\beta\colon (0, +\infty) \to \mathbb{C}$ has *rotated bounded variation* with phase ϕ if $e^{i\phi x}\beta(x)$ has bounded variation. A function $V\colon (0, +\infty) \to \mathbb{C}$ has *generalized bounded variation* with the set of phases $A = \{\phi_1, \dots, \phi_L\}$ if it can be expressed as a sum

$$V(x) = \sum_{l=1}^{L} \beta_l(x) + W(x) \tag{4.1.7}$$

such that the l-th function β_l has rotated bounded variation with phase ϕ_l and $W(x) \in L^1(x_0, +\infty)$. The set of functions having generalized bounded variation with the set of phases A will be denoted by $GBV(A)$ or $GBV(\phi_1, \dots, \phi_L)$.

The results mentioned above are just the ones that directly motivated our research, but there are many other related results. For example, Stolz [66] takes δ to be the forward difference operator $(\delta x)_n = x_{n+1} - x_n$ and analyzes Jacobi matrices with $a_n \equiv 1$ and $\delta^j b \in \ell^{k/j}$ for $1 \le j \le k$, showing that a.c. spectrum persists precisely on the interval $[-2 + \limsup_{n\to\infty} b_n, 2 + \liminf_{n\to\infty} b_n]$. In another direction, one can relax the bounded variation condition to an ℓ^2 condition on q-variation, namely $\sum_n |x_{n+q} - x_n|^2 < \infty$. Work by Denisov [15], extended by Kaluzhny–Shamis [36], has shown that this kind of perturbation with $x_n \to 0$ preserves the a.c. spectrum of periodic Jacobi operators.

All the results discussed so far concern perturbation of the free operator by generalized bounded variation. For perturbations of other operators, the situation is more complicated. For instance, in contrast to Weidmann's theorem, Last [40] has shown that for some classes of potentials V_0, perturbing the discrete Schrödinger operator $-\Delta + V_0$ by a perturbation V of bounded variation can destroy a.c. spectrum.

As communicated to us by Yoram Last, this problem can also be motivated in a different way: let $V_n = \lambda_n W_n$, with $\lambda_n > 0$ monotone decaying to 0, and let H be given by (4.2.3). For different classes of potentials W, what kind of decay do we need to ensure preservation of a.c. spectrum? If $\{\lambda_n\}$ is periodic, the method of Golinskii–Nevai [26] shows that any such $\{\lambda_n\}$ suffices. For W from a large class of random potentials, Kiselev–Last–Simon [38] have shown that $\{\lambda_n\} \in \ell^2$ is needed. For almost periodic potentials W which are trigonometric polynomials, we will provide an answer in Corollary 4.2.4.

4.2 New results

We now state the results that form the core of this thesis. The statements will use the concept of generalized bounded variation from Definitions 4.1.1 and 4.1.2.

Our first result is about orthogonal polynomials on the unit circle.

Theorem 4.2.1. *Let $d\mu = w(e^{i\theta})\frac{d\theta}{2\pi} + d\mu_{\mathrm{s}}$ be a probability measure on $\partial\mathbb{D}$ with infinite support and $\{\alpha_n\}_{n=0}^\infty$ its Verblunsky coefficients. Assume that*

$$\{\alpha_n\}_{n=0}^\infty \in \ell^p \cap GBV(A)$$

for a positive odd integer $p = 2q+1$ and a finite set $A \subset \mathbb{R}$. Let S be the finite set

$$S = \left\{ e^{i\eta} \;\middle|\; \eta \in (\underbrace{A + \cdots + A}_{q \text{ times}}) - (\underbrace{A + \cdots + A}_{q-1 \text{ times}}) \right\} \tag{4.2.1}$$

Then

(i) $\operatorname{supp}\mu_{\mathrm{s}} \subset S$ *and, in particular, $d\mu$ has no singular continuous part;*

(ii) $w(e^{i\theta})$ is continuous and strictly positive on $\partial\mathbb{D} \setminus S$.

The second theorem is the analogous result for orthogonal polynomials on the real line.

Theorem 4.2.2. *Let $d\rho = f(x)dx + d\rho_{\mathrm{s}}$ be a probability measure on the real line with infinite support and finite moments and $\{a_n, b_n\}_{n=1}^\infty$ its Jacobi coefficients. Let p be a positive integer, $A \subset \mathbb{R}$ a finite set of phases, and make one of these sets of assumptions:*

1° $\{a_n^2 - 1\}_{n=1}^\infty, \{b_n\}_{n=1}^\infty \in \ell^p \cap GBV(A)$

2° $\{a_n - 1\}_{n=1}^\infty, \{b_n\}_{n=1}^\infty \in \ell^p \cap GBV(A)$

Denote $\tilde{A} = A \cup \{0\}$ in case 1° and $\tilde{A} = (A + A) \cup A \cup \{0\}$ in case 2°, and let S be the finite set

$$S = \big\{ 2\cos(\eta/2) \bigm| \eta \in \underbrace{\tilde{A} + \cdots + \tilde{A}}_{p-1 \text{ times}} \big\} \tag{4.2.2}$$

Then

(i) $\operatorname{supp} \rho_{\mathrm{s}} \cap (-2, 2) \subset S$ *and, in particular, $d\rho$ has no singular continuous part;*

(ii) $f(x)$ is continuous and strictly positive on $(-2, 2) \setminus S$.

Remark 4.2.1. As we will see later, since recursion coefficients are in ℓ^p, all their constituent sequences of rotated bounded variation are in ℓ^p. However, if some of these constituent sequences have faster decay, this can be used to reduce the set S. Namely, a phase $\phi_1 + \cdots + \phi_k - \phi_{k+1} - \cdots - \phi_{k+l}$ must only be included in (4.2.1) or (4.2.2) if the pointwise product of the corresponding sequences, $\{\beta_n^{(1)} \cdots \beta_n^{(k)} \bar{\beta}_n^{(k+1)} \cdots \bar{\beta}_n^{(k+l)}\}$, is not in ℓ^1. The proofs of Theorems 4.2.1 and 4.2.2 in this text can be easily modified to show this.

Remark 4.2.2. By Lemma 4.3.2(vi) shown later in this text,

$$\{a_n - 1\}_{n=1}^\infty \in GBV(A) \implies \{a_n^2 - 1\}_{n=1}^\infty \in GBV((A + A) \cup A)$$

Also, $\{a_n - 1\}_{n=1}^\infty \in \ell^p$ implies $\{a_n^2 - 1\}_{n=1}^\infty \in \ell^p$. Thus, with the replacement of the set A by $(A + A) \cup A$, case 1° of Theorem 4.2.2 implies case 2°. For that reason, in the remainder of the text we will only discuss case 1° of Theorem 4.2.2. Case 2° was provided only because, to a spectral theorist, it seems like a more natural condition.

Remark 4.2.3. If a sequence $\{\beta_n\}$ has rotated q-bounded variation, i.e. $\sum |e^{i\phi}\beta_{n+q} - \beta_n| < \infty$, then it also has generalized bounded variation by Lemma 4.3.1(ii), so our results trivially extend to such sequences.

Theorem 4.2.2 can be viewed in the special case $a_n \equiv 1$, where it becomes a result on discrete Schrödinger operators on a half-line. Using a standard pasting argument, this also implies a result for discrete Schrödinger operators on a line.

Corollary 4.2.3. *Let*

$$(Hx)_n = x_{n+1} + V_n x_n + x_{n-1} \tag{4.2.3}$$

be a discrete Schrödinger operator on a half-line or line (with an arbitrary boundary condition if on a half-line), with $\{V_n\}$ *in* ℓ^p *with generalized bounded variation with set of phases* A*. Then*

(i) $\sigma_{\mathrm{ac}}(H) = [-2, 2]$

(ii) $\sigma_{\mathrm{sc}}(H) = \emptyset$

(iii) $\sigma_{\mathrm{pp}}(H) \cap (-2, 2)$ *is a finite set,*

$$\sigma_{\mathrm{pp}}(H) \cap (-2,2) \subset \left\{ 2\cos(\eta/2) \;\middle|\; \eta \in \bigcup_{k=1}^{p-1} (\underbrace{A + \cdots + A}_{k \text{ times}}) \right\}$$

This corollary applies in particular to linear combinations of Wigner–von Neumann potentials (4.1.4).

We single out the following case because it can be seen through the lens of almost periodic potentials. Namely, it shows that for a large class of almost periodic potentials, multiplying them by ℓ^p decay with any $p < \infty$ recovers the a.c. spectrum of the free operator.

Corollary 4.2.4. *Let*

$$(Hx)_n = x_{n+1} + \lambda_n W_n x_n + x_{n-1} \tag{4.2.4}$$

be a discrete Schrödinger operator on a half-line or line with $\{\lambda_n\} \in \ell^p$ *of bounded variation (with* $p < \infty$*) and* W *a trigonometric polynomial,*

$$W_n = \sum_{l=1}^{L} a_l \cos(2\pi\alpha_l n + \phi_l)$$

Then with $A = \{\pm 2\pi\alpha_1, \ldots, \pm 2\pi\alpha_l\}$*, all conclusions of Corollary 4.2.3 hold.*

Finally, we have results for Schrödinger operators. Our first result concerns Schrödinger operators on a half-line with potentials of generalized bounded variation at infinity.

Theorem 4.2.5. *Let* $H = -\Delta + V$ *be a Schrödinger operator on* $(0, \infty)$ *with* $V \in L^1_{\mathrm{loc}}(0, \infty)$ *such that*

(1) $V\colon (1, \infty) \to \mathbb{R}$ *has generalized bounded variation with an even set of phases* A*, i.e.*

$$V(x) = \sum_{l=1}^{L} \beta_l(x) + W(x) \tag{4.2.5}$$

where β_l *has rotated bounded variation with phase* $\phi_l \in A$ *and* $W \in L^1(1, \infty)$*;*

(2) $\beta_l \in L^p$ *for some* $p \in [1, \infty)$ *independent of* l*;*

(3) the operator $-\Delta + V$*, seen as a Schrödinger operator on the interval* $(0,1)$*, has purely discrete spectrum.*

Then the spectrum of H *is described by*

(i) $\sigma_{\mathrm{ac}}(H) = [0, \infty)$

(ii) $\sigma_{\mathrm{sc}}(H) = \emptyset$

(iii) $\sigma_{\mathrm{pp}}(H) \cap (0, \infty)$ *is a finite set,*

$$\sigma_{\mathrm{pp}}(H) \cap (0,\infty) \subset \left\{ \frac{\eta^2}{4} \,\middle|\, \eta \in \bigcup_{k=1}^{p-1} (\underbrace{A + \cdots + A}_{k \text{ times}}) \right\}$$

Note that assumption (3) is satisfied under very mild asymptotic conditions for V around 0, for example those in Theorem 3.3.4.

For a spherically symmetric potential $V(|x|)$ on $\mathbb{R}^n$, we saw in Section 3.5 that under certain conditions $H = -\Delta + V$ can be decomposed as a direct sum of half-line potentials

$$H_j = -\Delta + V(x) + \Big(\mu_j + \frac{(n-1)(n-3)}{4}\Big)\frac{1}{x^2}$$

where $\mu_j = j(j + n - 2)$. Note that

$$\Big(\mu_j + \frac{(n-1)(n-3)}{4}\Big)\frac{1}{x^2} \in L^1(1, \infty)$$

so this term doesn't affect the generalized bounded variation condition. Therefore, as long as the decomposition into half-line operators holds and the half-line operators obey the condition (3) of Theorem 4.2.5 at the origin, we will have a description of the spectrum of the spherically symmetric operator.

The remainder of this chapter is dedicated to proofs of Theorems 4.2.1, 4.2.2, and 4.2.5.

4.3 Proof of Theorems 4.2.1 and 4.2.2

In this section, we will present a proof of Theorems 4.2.1 and 4.2.2. We start by discussing some properties of sequences of generalized bounded variation in Subsection 1. Subsection 2 will set up the framework for both OPRL and OPUC in a unified way, which will enable us to present a shared proof of the two theorems. In Subsections 3 and 4 we present proofs of the two theorems in the ℓ^2 and ℓ^3 cases, building up the tools for the general proof in Subsections 5 and 6.

4.3.1 Sequences of generalized bounded variation

In this subsection we describe some properties of sequences of rotated and generalized bounded variation. Most importantly, we prove that if a sequence is of generalized bounded variation and is in some ℓ^p space, then all the constituent sequences are also in ℓ^p.

Lemma 4.3.1. (i) *Let $\alpha \in GBV(\phi_1, \dots, \phi_L)$, with decomposition* (4.1.3) *into sequences of rotated bounded variation. Then for any $1 \le p \le \infty$,*

$$\alpha \in \ell^p \implies \beta^{(1)}, \dots, \beta^{(L)} \in \ell^p$$

(ii) *If $\sum_n |e^{i\phi}\alpha_{n+q} - \alpha_n| < \infty$, then $\alpha \in GBV(\frac{\phi}{q}, \frac{\phi}{q} + \frac{2\pi}{q}, \dots, \frac{\phi}{q} + \frac{2(q-1)\pi}{q})$.*

Proof. (i) We will prove $\beta^{(1)} \in \ell^p$; the proof for any $\beta^{(l)}$ is analogous. Let T be the shift operator on sequences, defined by $Tz = \{z_{n+1}\}_{n=N}^\infty$ for $z = \{z_n\}_{n=N}^\infty$. In terms of T, the condition (4.1.2) can be rewritten as

$$(e^{i\phi_l}T - 1)\beta^{(l)} \in \ell^1 \tag{4.3.1}$$

Note that for any $1 \le q \le \infty$, $z \in \ell^q$ implies $Tz \in \ell^q$; thus, for an arbitrary polynomial $P(T)$,

$$z \in \ell^q \implies P(T)z \in \ell^q \tag{4.3.2}$$

Now let $Q(T) = \prod_{l=2}^L (e^{i\phi_l}T - 1)$. By (4.3.2) with $q = 1$, (4.3.1) implies $Q(T)\beta^{(l)} \in \ell^1$ for $l \ne 1$. Meanwhile, $\alpha \in \ell^p$ and (4.3.2) imply $Q(T)\alpha \in \ell^p$. Thus, applying $Q(T)$ to (4.1.3) gives

$$Q(T)\beta^{(1)} = Q(T)\alpha - \sum_{l=2}^L Q(T)\beta^{(l)} \ \in \ell^p \tag{4.3.3}$$

Since the ϕ_l are mutually distinct, $Q(T)$ is coprime with $e^{i\phi_1}T - 1$, so there exist complex polynomials $U(T), V(T)$ such that

$$1 = U(T)Q(T) + V(T)(e^{i\phi_1}T - 1)$$

Thus, applying $U(T)$ to (4.3.3) and $V(T)$ to $(e^{i\phi_1}T - 1)\beta^{(1)} \in \ell^1$ and adding the two, we obtain $\beta^{(1)} \in \ell^p$.

(ii) Let $R_k(T) = (e^{i\phi}T^q - 1)/(e^{i(\phi+2k\pi)/q}T - 1)$ for $0 \le k \le q-1$. Since there exist complex polynomials $U_k(T)$ with $1 = \sum_{k=0}^{q-1} R_k(T)U_k(T)$, by defining $\beta^{(k)} = R_k(T)U_k(T)\alpha$ one gets the required representation $\alpha = \sum_{k=0}^{q-1} \beta^{(k)}$ with $(e^{i(\phi+2k\pi)/q}T - 1)\beta^{(k)} \in \ell^1$. □

Remark 4.3.1. If a sequence α is of generalized bounded variation, uniqueness of the representation (4.1.3) is of some interest. Clearly, we can freely add ℓ^1 sequences to $\beta^{(l)}$'s, as long as the sum of those sequences cancels out in α. By doing so, we can eliminate any extraneous $\beta^{(l)}$ which are in ℓ^1.

Conversely, if we find a different representation $\alpha_n = \sum \tilde{\beta}_n^{(k)}$, then subtracting it from the representation (4.1.3) and applying Lemma 4.3.1 with $p = 1$, we see that to each $\beta^{(l)} \notin \ell^1$ there corresponds a unique $\tilde{\beta}^{(k)}$ with the same phase, such that their difference is an ℓ^1 sequence.

The following lemma describes some properties of sequences of generalized bounded variation. In particular, it shows that real sequences of generalized bounded variation have, in essence, an even set of phases and a symmetric representation with respect to complex conjugation.

Lemma 4.3.2. *Let $\phi, \psi \in \mathbb{R}$, $A, B, C \subset \mathbb{R}$, and $\beta = \{\beta_n\}_{n=N}^{\infty}$, $\gamma = \{\gamma_n\}_{n=N}^{\infty}$ (with N finite) complex sequences. Then*

(i) *If $\beta \in GBV(\phi)$, then β is bounded.*

(ii) *If $\beta \in GBV(\phi)$, $\gamma \in GBV(\psi)$, then $\{\beta_n\gamma_n\}_{n=N}^{\infty} \in GBV(\phi + \psi)$.*

(iii) *If $\beta \in GBV(B)$, $\gamma \in GBV(C)$, then $\{\beta_n\gamma_n\}_{n=N}^{\infty} \in GBV(B + C)$.*

(iv) *If $\beta \in GBV(B)$, $\gamma \in GBV(C)$, then $\{\beta_n + \gamma_n\}_{n=N}^{\infty} \in GBV(B \cup C)$.*

(v) *If $\beta \in GBV(B)$, then $\bar{\beta} \in GBV(-B)$.*

(vi) *If $\{a_n - 1\}_{n=1}^{\infty} \in GBV(A)$, then $\{a_n^2 - 1\}_{n=1}^{\infty} \in GBV((A + A) \cup A)$.*

(vii) *If $x \in GBV(A)$ with $x_n \in \mathbb{R}$, then x admits a representation*

$$x = \sum_{l=1}^{L} (\beta^{(l)} + \bar{\beta}^{(l)})$$

with $\beta^{(l)} \in GBV(\phi_l)$, such that $\phi_l \in A$ and for every $\beta^{(l)} \notin \ell^1$, the corresponding ϕ_l is in $-A + 2\pi\mathbb{Z}$.

Proof. (i) follows from the triangle inequality,

$$\begin{aligned} |\beta_n| &\leq |e^{iN\phi}\beta_N| + \sum_{m=N}^{n-1} |e^{i(m+1)\phi}\beta_{m+1} - e^{im\phi}\beta_m| \\ &\leq |\beta_N| + \sum_{m=N}^{\infty} |e^{i\phi}\beta_{m+1} - \beta_m| \end{aligned}$$

(ii) follows from the triangle inequality and part (i),

$$\begin{aligned} \left|e^{i(\phi+\psi)}\beta_{n+1}\gamma_{n+1} - \beta_n\gamma_n\right| &\leq \left|e^{i\psi}\gamma_{n+1}(e^{i\phi}\beta_{n+1} - \beta_n)\right| + \left|\beta_n(e^{i\psi}\gamma_{n+1} - \gamma_n)\right| \\ &\leq \|\gamma\|_\infty \left|e^{i\phi}\beta_{n+1} - \beta_n\right| + \|\beta\|_\infty \left|e^{i\psi}\gamma_{n+1} - \gamma_n\right| \end{aligned}$$

after summing over n.

(iii) is proved by decomposing β and γ into sequences of rotated bounded variation and applying (ii).

(iv) and (v) follow directly from Definition 4.1.1.

(vi) follows from (iii) and (iv), using $a_n^2 - 1 = (a_n - 1)^2 + 2(a_n - 1)$.

(vii) Taking an arbitrary representation of x and averaging it with its complex conjugate produces the desired form. Since $x = \bar{x}$, the other claim follows from (v) and Remark 4.3.1. □

4.3.2 Equisummability

In this subsection, we restate the problem in terms of Prüfer variables. We will be able to restate the problem for both OPRL and OPUC in a unified way, which will enable us to prove both theorems at once in the remainder of the section. Define a constant c,

$$c = \begin{cases} 0, & \text{for OPUC} \\ 1, & \text{for OPRL} \end{cases} \tag{4.3.4}$$

With Prüfer variables as defined in Sections 2.4 and 2.5, (2.4.5) and (2.5.4) can be written in a unified way as

$$\frac{r_{n+1}}{r_n} e^{i(\theta_{n+1}-\theta_n)} = \frac{1 - c\alpha_n - \bar{\alpha}_n e^{-i[(n+1)\eta+2\theta_n]}}{\sqrt{(1-c\alpha_n)(1-c\bar{\alpha}_n) - \alpha_n\bar{\alpha}_n}} \tag{4.3.5}$$

Taking the absolute value of this equation, or dividing it by its complex conjugate, we get

$$\frac{r_{n+1}}{r_n} = \frac{|1 - \alpha_n e^{i[(n+1)\eta+2\theta_n]} - c\bar{\alpha}_n|}{\sqrt{(1-c\alpha_n)(1-c\bar{\alpha}_n) - \alpha_n\bar{\alpha}_n}} \tag{4.3.6}$$

$$e^{2i(\theta_{n+1}-\theta_n)} = \frac{1 - \bar{\alpha}_n e^{-i[(n+1)\eta+2\theta_n]} - c\alpha_n}{1 - \alpha_n e^{i[(n+1)\eta+2\theta_n]} - c\bar{\alpha}_n} \tag{4.3.7}$$

For OPRL, by decomposing $a_n^2 - 1$ and b_n into sequences of rotated bounded variation, $\alpha_n(\eta)$ can be written as

$$\alpha_n(\eta) = \sum_{l=1}^{L} h_l(\eta)\beta_n^{(l)} \tag{4.3.8}$$

where $\beta^{(l)}$ has rotated bounded variation with phase ϕ_l and $h_l(\eta)$ are continuous non-vanishing functions on $(0, 2\pi)$. In fact, $h_l(\eta)$ are either $1/(e^{i\eta} - 1)$ or $e^{i\eta/2}/(e^{i\eta} - 1)$, depending on whether the corresponding $\beta^{(l)}$ was a part of $\{a_n^2 - 1\}_{n=1}^\infty$ or $\{b_n\}_{n=1}^\infty$. Further, if $\{a_n^2 - 1\}_{n=1}^\infty, \{b_n\}_{n=1}^\infty \in \ell^p$, then $\beta^{(l)} \in \ell^p$ by Lemma 4.3.1.

Note that unlike in OPUC, an arbitrary choice of sequences $\beta^{(l)} \in \ell^p \cap GBV(\phi_l)$ wouldn't correspond via (4.3.8) to a valid set of Jacobi parameters; rather, by Lemma 4.3.2(vii), up to an ℓ^1 term, for each $\beta^{(l)}$, its complex conjugate is also one of the sequences in (4.3.8).

Thus, for both OPUC and OPRL, the sequence $\alpha(\eta)$ can be written as

$$\alpha_n(\eta) = \sum_{l=1}^{L} h_l(\eta)\beta_n^{(l)} \tag{4.3.9}$$

where $\beta^{(l)}$ has rotated bounded variation with phase ϕ_l, $\beta^{(l)} \in \ell^p$ and $h_l(\eta)$ are continuous non-vanishing functions away from $A_1 + 2\pi\mathbb{Z}$, with

$$A_1 = \begin{cases} \emptyset, & \text{for OPUC} \\ \{0\}, & \text{for OPRL} \end{cases} \tag{4.3.10}$$

For a given set of phases, A, we will now define sets A_p with p a positive integer. Let

$$A_2 = A \cup A_1 \tag{4.3.11}$$

Let $q = \lceil (p-1)/2 \rceil$ (the smallest integer not smaller than $(p-1)/2$) and

$$A_p = \begin{cases} (\underbrace{A + \cdots + A}_{q \text{ times}}) - (\underbrace{A + \cdots + A}_{q-1 \text{ times}}), & \text{for OPUC} \\ \underbrace{A_2 + \cdots + A_2}_{p-1 \text{ times}}, & \text{for OPRL} \end{cases} \tag{4.3.12}$$

For OPRL, note that Lemma 4.3.2(vii) implies $A = -A$, and that $0 \in A_2$, so the set A_p contains all elements of

$$(\underbrace{A + \cdots + A}_{i \text{ times}}) - (\underbrace{A + \cdots + A}_{j \text{ times}})$$

for any $i \geq 1$, $j \geq 0$ and $i + j < p$. For OPUC, it only contains those with $i = j + 1$.

Definition 4.3.1. Let $B \subset \mathbb{R}$ be a finite set. We define *equisummability away from B*, a binary relation $\sim_B$ on the set of sequences parametrized by $\eta \in \mathbb{R}$, by: $u_n(\eta) \sim_B v_n(\eta)$ if and only if

$$\sum_{n=0}^{\infty} \big(u_n(\eta) - v_n(\eta)\big)$$

converges uniformly (but not necessarily absolutely) in $\eta \in I$ for intervals I with $\operatorname{dist}(I, B+2\pi\mathbb{Z}) > 0$.

We can now state a unified criterion for Theorems 4.2.1 and 4.2.2. We will need to reparametrize Prüfer variables: for OPUC, we will consider them as parameters of η instead of $z = e^{i\eta}$ and for OPRL, we will consider them parameters of η instead of $x = 2\cos(\eta/2)$.

Lemma 4.3.3. *Assume that all the assumptions of either Theorem 4.2.1 or 4.2.2 hold.*

(i) If

$$\log \frac{r_{n+1}(\eta)}{r_n(\eta)} \sim_{A_p} 0 \tag{4.3.13}$$

then all the conclusions of the corresponding theorem hold.

(ii) It is not possible to have $\log r_n(\eta)$ *converge uniformly to* $\pm\infty$ *for* η *in some interval* $I \subset \mathbb{R}$.

Note that this lemma is just a restatement of Lemmas 2.4.2 and 2.5.3.

4.3.3 Proof in the ℓ^2 case

In this subsection, we present a proof of (4.3.13) in the ℓ^2 case. We focus on this case in order to motivate elements of the proof of the general case and, in particular, a key lemma. We remind the reader that for OPUC, the ℓ^2 case has already been proved by Wong [80].

Taking the log of (4.3.6) and expanding to linear order in α_n, we get

$$\log \frac{r_{n+1}}{r_n} = -\operatorname{Re} \alpha_n e^{i[(n+1)\eta+2\theta_n]} + O(|\alpha_n|^2)$$

In the ℓ^2 case $O(|\alpha_n|^2) \sim_{A_1} 0$, so using (4.3.9),

$$\log \frac{r_{n+1}}{r_n} \sim_{A_1} -\operatorname{Re} \sum_{l=1}^{L} h_l(\eta) \beta_n^{(l)} e^{i[(n+1)\eta+2\theta_n]} \tag{4.3.14}$$

Now we need a way to control terms of the form $f(\eta)\Gamma_n e^{i[(n+1)\eta+2\theta_n]}$, with $\{\Gamma_n\}$ of rotated bounded variation with phase ϕ. But first we must take care of some prerequisites. We will need the function

$$\chi(\eta) = \frac{1}{e^{-i\eta}-1} = -\frac{1}{2} + \frac{i}{2}\cot\frac{\eta}{2} \tag{4.3.15}$$

Taylor expansions of (4.3.7) will turn out to be important: taking the k-th power of (4.3.7) and expanding in powers of α_n, we have

$$e^{2ki(\theta_{n+1}-\theta_n)} - 1 = P_{k,l}(\alpha_n, e^{i[(n+1)\eta+2\theta_n]}) + O(|\alpha_n|^l) \tag{4.3.16}$$

where

$$\begin{aligned} P_{k,l}(\alpha_n, e^{i[(n+1)\eta+2\theta_n]}) = \sum_{\substack{u,v\geq 0 \\ 0<u+v<l}} \Big((-1)^v \tbinom{k+u-1}{u} \tbinom{k}{v} [\alpha_n e^{i[(n+1)\eta+2\theta_n]} + c\bar{\alpha}_n]^u \\ \times [\bar{\alpha}_n e^{-i[(n+1)\eta+2\theta_n]} + c\alpha_n]^v \Big) \end{aligned} \tag{4.3.17}$$

The first part of the following lemma will give us a way of passing from a sequence of the form

$f(\eta)\Gamma_n e^{i[(n+1)\eta+2\theta_n]}$ to a faster decaying sequence, but at a cost of a multiplicative factor with possibly finitely many singularities. These singularities exactly correspond to the points where we can't rule out existence of a pure point. The main idea of the proof is that for η away from ϕ, the exponential factor $e^{in\eta}$ in this sequence helps average out parts of it when partial sums are taken.

The second part of the lemma uses the ℓ^p condition and shows that it is allowed to replace an appearance of $e^{2ik(\theta_{n+1}-\theta_n)} - 1$ by its Taylor polynomial $P_{k,l}$ of a sufficient power.

Lemma 4.3.4. *Let $k \in \mathbb{Z}$ and $\phi \in [0, 2\pi)$, with k and ϕ not both equal to 0. Let $B \subset \mathbb{R}$ be a finite set and $f\colon \mathbb{R} \setminus (B + 2\pi\mathbb{Z}) \to \mathbb{C}$ be a continuous function such that $g(\eta) = f(\eta)\chi(k\eta - \phi)$ is also continuous on $\mathbb{R} \setminus (B + 2\pi\mathbb{Z})$ (removable singularities in g are allowed).*

If $\{\Gamma_n\}$ has rotated bounded variation with phase ϕ and $\Gamma_n \to 0$, then

$$f(\eta)\Gamma_n e^{ik[(n+1)\eta+2\theta_n]} \sim_B g(\eta)\Gamma_n e^{ik[(n+1)\eta+2\theta_n]}\big(e^{2ik(\theta_{n+1}-\theta_n)} - 1\big) \tag{4.3.18}$$

In particular, let $\Gamma_n = \beta_n^{(k_1)} \cdots \beta_n^{(k_s)} \bar{\beta}_n^{(l_1)} \cdots \bar{\beta}_n^{(l_t)}$ with $\phi = \phi_{k_1} + \cdots + \phi_{k_s} - \phi_{l_1} - \cdots - \phi_{l_t}$. If all $\beta^{(j)} \in \ell^p$ and $A_1 \subset B$, then

$$f(\eta)\Gamma_n e^{ik[(n+1)\eta+2\theta_n]} \sim_B g(\eta)\Gamma_n e^{ik[(n+1)\eta+2\theta_n]} P_{k,p-s-t}(\alpha_n, e^{i[(n+1)\eta+2\theta_n]}) \tag{4.3.19}$$

Proof. Start by substituting $f(\eta) = g(\eta)(e^{-i(k\eta-\phi)} - 1)$,

$$\begin{aligned} f(\eta)\Gamma_n e^{ik[(n+1)\eta+2\theta_n]} &= g(\eta)(e^{-i(k\eta-\phi)} - 1)\Gamma_n e^{ik[(n+1)\eta+2\theta_n]} \\ &= g(\eta)\big(e^{i\phi}\Gamma_n e^{ik[n\eta+2\theta_n]} - \Gamma_n e^{ik[(n+1)\eta+2\theta_n]}\big) \end{aligned} \tag{4.3.20}$$

and note that $g(\eta)$ is bounded on intervals I with $\operatorname{dist}(I, B + 2\pi\mathbb{Z}) > 0$.

For a sequence $x_n(\eta)$ which converges to 0 uniformly in η away from $B + 2\pi\mathbb{Z}$,

$$\sum_{n=0}^{\infty}\big(x_n(\eta) - x_{n+1}(\eta)\big) = x_0(\eta)$$

uniformly in η, so $x_n(\eta) \sim_B x_{n+1}(\eta)$. Taking $x_n(\eta) = e^{i\phi}\Gamma_n e^{ik[n\eta+2\theta_n]}$ gives

$$e^{i\phi}\Gamma_n e^{ik[n\eta+2\theta_n]} \sim_B e^{i\phi}\Gamma_{n+1} e^{ik[(n+1)\eta+2\theta_{n+1}]} \tag{4.3.21}$$

Meanwhile, the rotated bounded variation condition for Γ_n implies

$$e^{i\phi}\Gamma_{n+1} e^{ik[(n+1)\eta+2\theta_{n+1}]} \sim_B \Gamma_n e^{ik[(n+1)\eta+2\theta_{n+1}]} \tag{4.3.22}$$

Applying (4.3.21) and then (4.3.22) to the first term of the right-hand side of (4.3.20) proves (4.3.18).

To prove (4.3.19), use Lemma 4.3.2(ii),(v) to note that Γ has rotated bounded variation with phase ϕ. Using (4.3.9) and continuity of $h_l(\eta)$ away from A_1, on an interval I with $\operatorname{dist}(I, A_1+2\pi\mathbb{Z}) > 0$ we have

$$|\alpha_n| \leq C_1 \sum_{l=1}^{L} |\beta_n^{(l)}| \tag{4.3.23}$$

for some constant C_1. Since $\beta^{(l)}$ are bounded sequences, $\alpha_n(\eta)$ is uniformly bounded for $\eta \in I$. Thus, (4.3.16) implies

$$\left| e^{2ki(\theta_{n+1}-\theta_n)} - 1 - P_{k,p-s-t}(\alpha_n, e^{i[(n+1)\eta+2\theta_n]}) \right| \leq C_2 |\alpha_n|^{p-s-t}$$

Combining this with (4.3.23) and $\Gamma_n = \beta_n^{(k_1)} \cdots \beta_n^{(k_s)} \bar{\beta}_n^{(l_1)} \cdots \bar{\beta}_n^{(l_t)}$, and using $\beta^{(j)} \in \ell^p$, we get

$$g(\eta)\Gamma_n e^{ik[(n+1)\eta+2\theta_n]} \left(e^{2ki(\theta_{n+1}-\theta_n)} - 1 - P_{k,p-s-t}(\alpha_n, e^{i[(n+1)\eta+2\theta_n]}) \right) \sim_B 0$$

Subtracting this from (4.3.18) gives (4.3.19) and completes the proof. □

Using this lemma, we can finish the proof for the ℓ^2 case. Notice that the factor $\chi(\eta - \phi_l)$ is continuous away from $\phi_l \in A_2$, and that $h_l(\eta)$ are continuous away from $A_1 \subset A_2$. Also, from (4.3.17) or (4.3.7), (4.3.16) we have $e^{2i(\theta_{n+1}-\theta_n)} - 1 = O(|\alpha_n|)$, i.e. $P_{1,1} = 0$, so by Lemma 4.3.4,

$$h_l(\eta)\beta_n^{(l)} e^{i[(n+1)\eta+2\theta_n]} \sim_{A_2} 0 \tag{4.3.24}$$

Summing this over l and combining into (4.3.14) finally gives

$$\log \frac{r_{n+1}}{r_n} \sim_{A_2} 0$$

which completes the proof.

4.3.4 Proof in the ℓ^3 case

In this subsection, we present the proof in the ℓ^3 case to provide further motivation for the general proof. Beyond ℓ^2, Lemma 4.3.4 needs to be used iteratively, and the ℓ^3 case illustrates the difficulties encountered in performing this iterative procedure.

Taking the log of (4.3.6) and expanding in powers of α_n, then using $O(|\alpha_n|^3) \sim_{A_1} 0$ implies

$$\log \frac{r_{n+1}}{r_n} \sim_{A_1} \operatorname{Re}\left(-\alpha_n e^{i[(n+1)\eta+2\theta_n]} - \tfrac{1}{2}\alpha_n^2 e^{2i[(n+1)\eta+2\theta_n]} - c\alpha_n\bar{\alpha}_n e^{i[(n+1)\eta+2\theta_n]} + \tfrac{1}{2}\alpha_n\bar{\alpha}_n \right) \tag{4.3.25}$$

As in the ℓ^2 case, we now want to apply Lemma 4.3.4 to parts of this expression. We begin with the first-order term in α_n. In the ℓ^2 case, using (4.3.9) to break up α_n and using Lemma 4.3.4 gave

(4.3.24). However, applying the same lemma in the ℓ^3 case, we need $P_{1,2}$ instead of $P_{1,1}$, since terms quadratic in the sequences $\beta^{(j)}$ cannot be automatically discarded. Thus, instead of (4.3.24) we get

$$h_l(\eta)\beta_n^{(l)}e^{i[(n+1)\eta+2\theta_n]} \sim_{A_2} h_l(\eta)\chi(\eta-\phi_l)\beta_n^{(l)}e^{i[(n+1)\eta+2\theta_n]}\big(-c\alpha_n + c\bar{\alpha}_n - \bar{\alpha}_n e^{-i[(n+1)\eta+2\theta_n]} + \alpha_n e^{i[(n+1)\eta+2\theta_n]}\big) \tag{4.3.26}$$

Note that all terms on the right-hand side contain a $\beta_n^{(l)}$ and an α_n or $\bar{\alpha}_n$, so we have obtained a faster decaying expression in n, although at the cost of a singularity at $\eta = \phi_l$.

Summing (4.3.26) over l and inserting into (4.3.25), and using (4.3.9) to replace α_n everywhere, we have

$$\log \frac{r_{n+1}}{r_n} \sim_{A_2} \operatorname{Re} \sum_{l,m=1}^{L} \big(X_{l,m} + Y_{l,m} + Z_{l,m} + T_{l,m}\big) \tag{4.3.27}$$

where

$$X_{l,m} = -\big(\tfrac{1}{2} + \chi(\eta-\phi_l)\big)h_l(\eta)h_m(\eta)\beta_n^{(l)}\beta_n^{(m)}e^{2i[(n+1)\eta+2\theta_n]} \tag{4.3.28}$$

$$Y_{l,m} = \big(\tfrac{1}{2} + \chi(\eta-\phi_l)\big)h_l(\eta)\bar{h}_m(\eta)\beta_n^{(l)}\bar{\beta}_n^{(m)} \tag{4.3.29}$$

$$Z_{l,m} = c\chi(\eta-\phi_l)h_l(\eta)h_m(\eta)\beta_n^{(l)}\beta_n^{(m)}e^{i[(n+1)\eta+2\theta_n]} \tag{4.3.30}$$

$$T_{l,m} = -c\big(1 + \chi(\eta-\phi_l)\big)h_l(\eta)\bar{h}_m(\eta)\beta_n^{(l)}\bar{\beta}_n^{(m)}e^{i[(n+1)\eta+2\theta_n]} \tag{4.3.31}$$

We proceed by applying Lemma 4.3.4 to these expressions.

For OPRL, since singularities of $\chi(\eta-\phi_l-\phi_m)$ and $\chi(\eta-\phi_l+\phi_m)$ are inside A_3, applying Lemma 4.3.4 we get

$$Z_{l,m} \sim_{A_3} 0 \tag{4.3.32}$$

$$T_{l,m} \sim_{A_3} 0 \tag{4.3.33}$$

The same formulas hold for OPUC, but for a different reason: $c = 0$ implies that $Z_{l,m} = T_{l,m} = 0$, so (4.3.32) and (4.3.33) are trivial. This is why for OPUC, $\phi_l + \phi_m$ and $\phi_l - \phi_m$ don't need to be included into A_3.

For $X_{l,m}$, Lemma 4.3.4 gives a multiplicative factor $\chi(2\eta-\phi_l-\phi_m)$, which has singularities at $\eta = (\phi_l+\phi_m)/2 + \pi\mathbb{Z}$. These points are not in A_3, so it might seem that we will have to apply Lemma 4.3.4 with a set greater than A_3. We are saved by the observation

$$\big(1 + \chi(\eta-\phi_l) + \chi(\eta-\phi_m)\big)\chi(2\eta-\phi_l-\phi_m) = \chi(\eta-\phi_l)\chi(\eta-\phi_m) \tag{4.3.34}$$

which is straightforward to check from (4.3.15). Thus, applying Lemma 4.3.4 to $X_{l,m} + X_{m,l}$, the points $\eta = (\phi_l + \phi_m)/2 + \pi\mathbb{Z}$ are just removable singularities in (4.3.34) and we get

$$X_{l,m} + X_{m,l} \sim_{A_2} 0 \tag{4.3.35}$$

Since (4.3.27) contains a sum over all l, m, this is sufficient for our purposes. Combining terms with different permutations of the same indices will also be used in the general case, to avoid unnecessarily expanding the set of critical points. Indeed, Subsection 4.3.5 generalizes the observation (4.3.34) to the general case.

If $\phi_l \neq \phi_m$, $\chi(\phi_m - \phi_l)$ is just a finite constant so Lemma 4.3.4 can be applied to $Y_{l,m}$ to give

$$Y_{l,m} \sim_{A_2} 0 \qquad (\text{if } \phi_l \neq \phi_m) \tag{4.3.36}$$

Combining (4.3.32), (4.3.33), (4.3.35) and (4.3.36) into (4.3.27), we have

$$\log \frac{r_{n+1}}{r_n} \sim_{A_3} \operatorname{Re} \sum_{\substack{1 \le l,m \le L \\ \phi_l = \phi_m}} Y_{l,m} \tag{4.3.37}$$

Lemma 4.3.4 is not applicable to the remaining $Y_{l,m}$'s, but we are again saved by an observation that

$$\operatorname{Re}\bigl(\tfrac{1}{2} + \chi(\eta - \phi_l)\bigr) = 0 \tag{4.3.38}$$

Because of this, when $\phi_l = \phi_m$,

$$\bar{Y}_{l,m} = -\bigl(\tfrac{1}{2} + \chi(\eta - \phi_l)\bigr)\bar{h}_l(\eta) h_m(\eta) \bar{\beta}_n^{(l)} \beta_n^{(m)} = -Y_{m,l}$$

so $\operatorname{Re}(Y_{l,m} + Y_{m,l}) = 0$ and (4.3.37) becomes

$$\log \frac{r_{n+1}}{r_n} \sim_{A_3} 0 \tag{4.3.39}$$

which completes the proof.

In the proof above the observation (4.3.38) was crucial. To try to arrive at a more illuminating proof, we will focus on OPUC (where $h_l(\eta) = 1$) and assume that instead of (4.3.37) we have, more generally,

$$\log \frac{r_{n+1}}{r_n} \sim_{A_3} \operatorname{Re} \sum_{\substack{1 \le l,m \le L \\ \phi_l = \phi_m}} f_l(\eta) \beta_n^{(l)} \bar{\beta}_n^{(m)} \tag{4.3.40}$$

We will now show that $\operatorname{Re} f_l(\eta) = 0$ for all l and η by proving that the converse leads to a contradiction with Lemma 4.3.3(ii).

Assume $\operatorname{Re} f_k(\eta_0) \neq 0$ for some k and η_0. Let

$$\beta_n^{(l)} = \begin{cases} e^{-in\phi_k}/(n+2)^{1/2} & \text{for } l = k \\ 0 & \text{else} \end{cases} \tag{4.3.41}$$

We have suppressed all $\beta^{(l)}$ with $l \neq k$. We have chosen $n+2$ in order to make all $|\beta_n^{(k)}| < 1$; note that this makes $\alpha_n = \beta_n^{(k)}$ an allowed choice of Verblunsky coefficients, corresponding by Verblunsky's theorem to a unique probability measure on the unit circle.

With the choice (4.3.41), (4.3.40) becomes

$$\log \frac{r_{n+1}}{r_n} \sim_{A_3} \operatorname{Re} f_k(\eta)/(n+2) \tag{4.3.42}$$

Since the harmonic series is divergent and $\operatorname{Re} f_k(\eta)$ is continuous in η, depending on the sign of $\operatorname{Re} f_k(\eta_0)$, summing (4.3.42) in n gives

$$\log r_n(\eta) \to \pm\infty$$

uniformly in a neighborhood of η_0. However, this is a contradiction with Lemma 4.3.3(ii). Thus, $\operatorname{Re} f_l(\eta) = 0$, so (4.3.40) becomes (4.3.39), which completes this alternative proof for OPUC. This method can be applied to OPRL as well, with one extra difficulty: $\beta^{(l)}$'s are not independent there, so in constructing counterexamples we have to be more careful than (4.3.41). Indeed, instead of relying on observations of the type (4.3.38), this will be the method we will apply to the general ℓ^p case in Subsection 4.3.6.

4.3.5 Narrowing the set of exceptional points

In the previous subsection, if we hadn't made the observation (4.3.34) telling us that $\eta = \frac{\phi_k + \phi_l}{2} + \pi\mathbb{Z}$ are removable singularities, we would have only proved equisummability away from a larger set of points, and we would have had a weaker result on the set of possible pure points. In this subsection, we generalize that observation to ℓ^p. In the ℓ^p case, iterations of Lemma 4.3.4 give multiplicative factors of the form

$$\chi\left(k\eta - \sum_{a=1}^{i} \phi_{m_a} + \sum_{b=1}^{j} \phi_{n_b}\right)$$

with $k \leq i$ and $i + j < p$. Such a factor has singularities at

$$\eta = \frac{1}{k}\left(\sum_{a=1}^{i} \phi_{m_a} - \sum_{b=1}^{j} \phi_{n_b}\right) + \frac{1}{k}\, 2\pi\mathbb{Z} \tag{4.3.43}$$

Surprisingly, with a more careful analysis shown in this subsection, all the singularities corresponding to $k \geq 2$ will turn into removable singularities where needed, so they don't have to be included into A_p.

The analysis that follows is quite technical, but the reader not interested in this aspect of the results may skip to the next subsection and replace the set A_p by a greater (but still finite) set, containing all elements of the form (4.3.43) with $k \leq i$ and $i + j < p$.

First let us set some conventions and definitions. We will use the Kronecker symbol δ_n which is 1 if $n = 0$ and 0 otherwise. Note that

$$\sum_{i=0}^{I} \delta_{i-k}\delta_{I-i-(K-k)} = \delta_{I-K} \tag{4.3.44}$$

We will use the combinatorial convention for binomial coefficients, i.e.

$$\binom{n}{k} = \begin{cases} \frac{n!}{k!(n-k)!} & \text{if } 0 \leq k \leq n \\ 0 & \text{else} \end{cases} \tag{4.3.45}$$

Two identities will be useful: for $l, m, n \geq 0$,

$$\sum_{k=0}^{l} \binom{m}{k}\binom{n}{l-k} = \binom{m+n}{l} \tag{4.3.46}$$

$$\sum_{k=0}^{l} \binom{m+k}{m}\binom{n+l-k}{n} = \binom{l+m+n+1}{m+n+1} \tag{4.3.47}$$

(4.3.46) is just Vandermonde's identity. The more obscure (4.3.47) has a combinatorial proof, by double-counting the number of subsets of $\{1, \ldots, l+n+m+1\}$ with exactly $m+n+1$ elements: observe that the number of such subsets whose $(m+1)$-st smallest element is $m+k+1$ is exactly $\binom{m+k}{m}\binom{n+l-k}{n}$.

We also need a kind of symmetrized product of functions:

Definition 4.3.2. For a function $p_{I,J}$ of $1 + I + J$ variables and a function $q_{K,L}$ of $1 + K + L$ variables, we define their symmetric product as a function $p_{I,J} \odot q_{K,L}$ of $1 + (I + K) + (J + L)$ variables by

$$(p_{I,J} \odot q_{K,L})\big(\eta; \{x_i\}_{i=1}^{I+K}; \{y_j\}_{j=1}^{J+L}\big) = \frac{1}{(I+K)!(J+L)!} \sum_{\substack{\sigma \in S_{I+K} \\ \tau \in S_{J+L}}} r_{\sigma,\tau}$$

with S_n the symmetric group in n elements and

$$r_{\sigma,\tau} = p_{I,J}\big(\eta; \{x_{\sigma(i)}\}_{i=1}^{I}; \{y_{\tau(j)}\}_{j=1}^{J}\big) q_{K,L}\big(\eta; \{x_{\sigma(i)}\}_{i=I+1}^{I+K}; \{y_{\tau(j)}\}_{j=J+1}^{J+L}\big)$$

It is straightforward to see that $\odot$ is commutative and associative.

Assuming we are in the ℓ^p case, we have $O(|\alpha_n|^p) \sim_{A_1} 0$, so expanding the log of (4.3.6) in powers of α_n gives

$$\log \frac{r_{n+1}}{r_n} \sim_{A_1} -\operatorname{Re} \sum_{\substack{K,L\geq 0\\ 0<K+L<p}} \tfrac{1}{K+L}\tbinom{K+L}{K}\big(\alpha_n e^{i[(n+1)\eta+2\theta_n]}\big)^K (c\bar\alpha_n)^L + \tfrac{1}{2} \sum_{\substack{k,l\geq 0\\ 0<k+2l<p}} \tfrac{1}{k+l}\tbinom{k+l}{k}(c\alpha_n + c\bar\alpha_n)^k \big((1-c^2)\alpha_n\bar\alpha_n\big)^l \tag{4.3.48}$$

Note that this is of the form

$$\log \frac{r_{n+1}}{r_n} \sim_{A_1} \operatorname{Re} \sum_{\substack{I,J,K,L\geq 0\\ I+J<p}} \xi_{I,J,K,L}\, \alpha_n^I \bar\alpha_n^J e^{iK[(n+1)\eta+2\theta_n]} c^L \tag{4.3.49}$$

where $\xi_{I,J,K,L}$ are constants. For $K > 0$ only the first sum in (4.3.48) contributes to $\xi_{I,J,K,L}$ and we read off their values,

$$\xi_{I,J,K,L} = \delta_{I-K}\delta_{J-L} \frac{1}{K+L}\binom{K+L}{K} \qquad (\text{for } K > 0) \tag{4.3.50}$$

(the values for $K = 0$ will turn out to be of no importance to us).

Our method is to substitute α_n using (4.3.9) and apply Lemma 4.3.4 to terms of the form

$$f(\eta) \prod_{i=1}^{I} (h_{k_i}(\eta)\beta_n^{(k_i)}) \prod_{j=1}^{J} (\bar h_{l_j}(\eta)\bar\beta_n^{(l_j)})\ e^{iK[(n+1)\eta+2\theta_n]}\ c^L \tag{4.3.51}$$

in increasing order of $I + J$. Note that this term will occur in all possible permutations of $k_1, \ldots, k_I$ and of $l_1, \ldots, l_J$, so we can average in those terms before applying Lemma 4.3.4. After such averaging, the function $f(\eta)$ in the term (4.3.51) is of the form

$$f_{I,J,K,L}(\eta; \phi_{k_1}, \ldots, \phi_{k_I}; \phi_{l_1}, \ldots, \phi_{l_J})$$

and the corresponding $g(\eta)$ constructed by Lemma 4.3.4 is

$$g_{I,J,K,L} = \chi\Big(K\eta - \sum_{i=1}^{I} \phi_{k_i} + \sum_{j=1}^{J} \phi_{l_j}\Big) f_{I,J,K,L} \tag{4.3.52}$$

All terms we encounter have $I, J, K, L \geq 0$, so we define

$$f_{I,J,K,L} = g_{I,J,K,L} = 0 \qquad \text{unless } I, J, K, L \geq 0 \tag{4.3.53}$$

Note that $f_{I,J,K,L}$ and $g_{I,J,K,L}$ are well-defined functions of $1+I+J$ parameters, and that they are symmetric in the I parameters ϕ_{k_i} and also in the J parameters ϕ_{l_j}. Our goal is precisely to show that $g_{I,J,K,L}$ has its singularities only at points of the form (4.3.43) with $k=1$. To do this, we will first establish a recurrence relation for these functions.

Any contribution to $f_{I,J,K,L}$ is either $\xi_{I,J,K,L}$ from the starting expression (4.3.49) or comes from an earlier term as $g_{\iota,j,k,l}$ multiplied by a constant from the Taylor expansion $P_{k,p-\iota-j}$ of $e^{2ik(\theta_{n+1}-\theta_n)}-1$. Starting from (4.3.17) and expanding, we have

$$P_{k,l}(\alpha_n, e^{i[(n+1)\eta+2\theta_n]}) = \sum_{\substack{\alpha,\beta,\gamma,\delta\geq 0\\ 0<\alpha+\beta+\gamma+\delta<l}} \Big((-1)^{\gamma+\delta}\tbinom{k+\alpha+\beta-1}{\alpha+\beta}\tbinom{\alpha+\beta}{\alpha}\tbinom{k}{\gamma+\delta}\tbinom{\gamma+\delta}{\gamma} \times (\alpha_n)^{\alpha+\delta}(\bar{\alpha}_n)^{\beta+\gamma}(e^{i[(n+1)\eta+2\theta_n]})^{\alpha-\gamma}c^{\beta+\delta}\Big) \tag{4.3.54}$$

From (4.3.54) we read off the value of the constant multiplying $g_{\iota,j,k,l}$, and matching the powers of α_n, $\bar{\alpha}_n$, $e^{i[(n+1)\eta+2\theta_n]}$, and c, we get $I=\iota+\alpha+\delta$, $J=j+\beta+\gamma$, $K=k+\alpha-\gamma$, $L=l+\beta+\delta$.

Since $f_{I,J,K,L}$ is then symmetrized in the appropriate variables, every product of $g_{\iota,j,k,l}$ by a constant becomes a symmetric product, so

$$f_{I,J,K,L} = \xi_{I,J,K,L} + \sum_{\substack{\alpha,\beta,\gamma,\delta\geq 0\\ \alpha+\beta+\gamma+\delta\geq 1}} \omega_{K,\alpha,\beta,\gamma,\delta}\odot g_{I-\alpha-\delta,J-\beta-\gamma,K+\gamma-\alpha,L-\beta-\delta} \tag{4.3.55}$$

with $\omega_{K,\alpha,\beta,\gamma,\delta}$ a constant function of $1+(\alpha+\delta)+(\beta+\gamma)$ variables,

$$\omega_{K,\alpha,\beta,\gamma,\delta} = (-1)^{\gamma+\delta}\tbinom{K+\gamma+\beta-1}{\alpha+\beta}\tbinom{K+\gamma-\alpha}{\gamma+\delta}\tbinom{\alpha+\beta}{\alpha}\tbinom{\gamma+\delta}{\gamma} \tag{4.3.56}$$

(this is the constant from (4.3.54), with the replacement $k=K+\gamma-\alpha$). By the convention (4.3.45), the right-hand side of (4.3.56) is 0 unless $K\geq 1$ and $\alpha,\beta,\gamma,\delta\geq 0$.

We have found the desired recursion relation in the form of (4.3.55). Note that (4.3.52), (4.3.53) and (4.3.55) determine the $f_{I,J,K,L}$ and $g_{I,J,K,L}$ uniquely.

Since $\omega_{K,0,0,0,0}=1$, it is convenient to define

$$h_{I,J,K,L} = f_{I,J,K,L} + g_{I,J,K,L} \tag{4.3.57}$$

and rewrite (4.3.55) as

$$h_{I,J,K,L} = \xi_{I,J,K,L} + \sum_{\alpha,\beta,\gamma,\delta\geq 0} \omega_{K,\alpha,\beta,\gamma,\delta}\odot g_{I-\alpha-\delta,J-\beta-\gamma,K+\gamma-\alpha,L-\beta-\delta} \tag{4.3.58}$$

Note that (4.3.57) and (4.3.52) imply

$$h_{I,J,K,L} = g_{I,J,K,L}\ \exp\Big(-i\big(K\eta - \sum_{i=1}^{I}\phi_{k_i} + \sum_{j=1}^{J}\phi_{l_j}\big)\Big) \tag{4.3.59}$$

It will be useful to introduce a rescaled version of functions introduced so far.

Define $\Omega_{K,\alpha,\beta,\gamma,\delta}$ as a function of $1+(\alpha+\delta)+(\beta+\gamma)$ variables,

$$\Omega_{K,\alpha,\beta,\gamma,\delta} = (-1)^{\gamma+\delta}\tbinom{K+\gamma+\beta-1}{K-1}\tbinom{K}{\alpha+\delta}\tbinom{\alpha+\delta}{\alpha}\tbinom{\beta+\gamma}{\beta} \tag{4.3.60}$$

By (4.3.45), this is equal to 0 unless $K \geq 1$ and $\alpha, \beta, \gamma, \delta \geq 0$.

Define $\Xi_{I,J,K,L}$ as a function of $1+I+J$ variables equal to

$$\Xi_{I,J,K,L} = \delta_{I-K}\delta_{J-L}\tbinom{K+L-1}{K-1} \tag{4.3.61}$$

By (4.3.45), this is equal to 0 unless $I = K \geq 1$ and $J = L \geq 0$.

It is straightforward to check

$$(K+\gamma-\alpha)\Omega_{K,\alpha,\beta,\gamma,\delta} = K\omega_{K,\alpha,\beta,\gamma,\delta} \tag{4.3.62}$$

$$\Xi_{I,J,K,L} = K\xi_{I,J,K,L} \tag{4.3.63}$$

so if we define

$$G_{I,J,K,L} = Kg_{I,J,K,L} \tag{4.3.64}$$

$$H_{I,J,K,L} = Kh_{I,J,K,L} \tag{4.3.65}$$

then multiplying (4.3.58) and (4.3.59) by K gives

$$H_{I,J,K,L} = \Xi_{I,J,K,L} + \sum_{\alpha,\beta,\gamma,\delta\geq 0}\Omega_{K,\alpha,\beta,\gamma,\delta}\odot G_{I-\alpha-\delta,J-\beta-\gamma,K+\gamma-\alpha,L-\beta-\delta} \tag{4.3.66}$$

$$H_{I,J,K,L} = G_{I,J,K,L}\ \exp\Big(-i\big(K\eta - \sum_{i=1}^{I}\phi_{k_i} + \sum_{j=1}^{J}\phi_{l_j}\big)\Big) \tag{4.3.67}$$

We are striving to prove the identity

$$\sum_{i,j,l\geq 0} G_{i,j,k,l}\odot G_{I-i,J-j,K-k,L-l} = \begin{cases} G_{I,J,K,L} & \text{if } 0 < k < K \\ 0 & \text{else} \end{cases} \tag{4.3.68}$$

Comparing with the ℓ^3 case, the observation (4.3.34) is a special case of this identity, namely,

$G_{2,0,2,0} = G_{1,0,1,0} \odot G_{1,0,1,0}$ (since $G_{0,0,1,0} = 0$ is easily computed from the recurrence relations).

The following lemma proves identity (4.3.68) and uses it to describe nonremovable singularities of $f_{I,J,K,L}$ and $g_{I,J,K,L}$. It also analyzes the case $L = 0$ in particular, since this is the only case that matters for OPUC ($c = 0$ means that (4.3.51) vanishes for $L > 0$).

Lemma 4.3.5. *For $I, J, K, L, k, A, B, C, D \in \mathbb{Z}$, the following are true:*

(i) *For $0 < k < K$,*

$$\sum_{i=0}^{I} \sum_{j=0}^{J} \sum_{l=0}^{L} \Xi_{i,j,k,l} \odot \Xi_{I-i,J-j,K-k,L-l} = \Xi_{I,J,K,L} \tag{4.3.69}$$

(ii) *For $0 < k < K$,*

$$\sum_{a=0}^{A} \sum_{b=0}^{B} \sum_{c=0}^{C} \sum_{d=0}^{D} \Omega_{K-k,A-a,B-b,C-c,D-d} \odot \Omega_{k,a,b,c,d} = \Omega_{K,A,B,C,D} \tag{4.3.70}$$

(iii) *For $k \geq 1$,*

$$\sum_{i,j,l \geq 0} \Xi_{i,j,k,l} \odot G_{I-i,J-j,K-k,L-l} = \sum_{\substack{\alpha,\beta,\gamma,\delta \geq 0 \\ \alpha \geq \gamma + k}} \Omega_{k,\alpha,\beta,\gamma,\delta} \odot G_{I-\alpha-\delta,J-\beta-\gamma,K+\gamma-\alpha,L-\beta-\delta} \tag{4.3.71}$$

(iv) (4.3.68) *holds for all $I, J, K, L \in \mathbb{Z}$.*

(v) *Nonremovable singularities of $f_{I,J,K,L}$ are of the form* (4.3.43) *with $k = 1$ and $i + j < I + J$.*

(vi) *Nonremovable singularities of $g_{I,J,K,L}$ are of the form* (4.3.43) *with $k = 1$ and $i + j \leq I + J$.*

(vii) *Nonremovable singularities of $f_{I,J,K,0}$ are of the form* (4.3.43) *with $k = i - j = 1$ and $i + j < I + J$.*

(viii) *Nonremovable singularities of $g_{I,J,K,0}$ are of the form* (4.3.43) *with $k = i - j = 1$ and $i + j \leq I + J$.*

Proof. (i) First note that both sides of (4.3.69) are zero unless $I, J, L \geq 0$. If $I, J, L \geq 0$, using the definition (4.3.61), (4.3.69) follows from a double application of (4.3.44) to resolve the sums in i and j, and (4.3.47) to resolve the sum in l.

(ii) First note that both sides of (4.3.70) are zero unless $A, B, C, D \geq 0$. If $A, B, C, D \geq 0$, using the definition (4.3.60), the left-hand side of (4.3.70) becomes a product of a sum in indices a and d and a sum in b and c.

For the sum in a and d, we introduce a change of indices to $x = a + d$ instead of d. The summand is 0 outside the limits of summation, so including some extra terms doesn't alter the sum, thus

$$\begin{aligned}\sum_{a=0}^{A}\sum_{d=0}^{D}\binom{K-k}{A+D-a-d}\binom{A+D-a-d}{A-a}\binom{k}{a+d}\binom{a+d}{a} &= \sum_{x=0}^{A+D}\sum_{a=0}^{x}\binom{K-k}{A+D-x}\binom{A+D-x}{A-a}\binom{k}{x}\binom{x}{a}\\ &= \sum_{x=0}^{A+D}\binom{K-k}{A+D-x}\binom{k}{x}\binom{A+D}{A}\\ &= \binom{K}{A+D}\binom{A+D}{A}\end{aligned}$$

after a double application of (4.3.46), first to compute the sum in a, and then the sum in x.

In the sum over b and c, we introduce a change of indices to $y = b + c$ instead of c. Analogously to the previous sum, since the summand is 0 outside the limits of summation,

$$\begin{aligned}\sum_{b=0}^{B}\sum_{c=0}^{C}\binom{K-k+B-b+C-c-1}{K-k-1}\binom{B+C-b-c}{B-b}\binom{k+c+b-1}{k-1}\binom{b+c}{b} &= \sum_{y=0}^{B+C}\sum_{b=0}^{y}\binom{K-k+B+C-y-1}{K-k-1}\binom{B+C-y}{B-b}\binom{k+y-1}{k-1}\binom{y}{b}\\ &= \sum_{y=0}^{B+C}\binom{K-k+B+C-y-1}{K-k-1}\binom{B+C}{B}\binom{k+y-1}{k-1}\\ &= \binom{K+B+C-1}{K-1}\binom{B+C}{B}\end{aligned}$$

where we have used (4.3.46) to compute the sum in b, then (4.3.47) to compute the sum in y.

Multiplying the two sums completes the proof of (4.3.70).

(iii) By (4.3.61), $\Xi_{i,j,k,l}$ is only nonzero if $i = k$ and $j = l$, so the left-hand side of (4.3.71) becomes just a sum over l,

$$\sum_{l\geq 0}\Xi_{k,l,k,l}\odot G_{I-k,J-l,K-k,L-l}$$

By (4.3.60), $\Omega_{k,\alpha,\beta,\gamma,\delta}$ has $\binom{k}{\alpha+\delta}$ as one of the factors, so it can only be nonzero if $\alpha+\delta \leq k$. Coupled with $\alpha \geq \gamma + k$ and $\gamma, \delta \geq 0$, this gives $\alpha = k$, $\gamma = \delta = 0$, so the right-hand side of (4.3.71) becomes

$$\sum_{\beta\geq 0}\Omega_{k,k,\beta,0,0}\odot G_{I-k,J-\beta,K-k,L-\beta}$$

The proof is completed by $\Xi_{k,\beta,k,\beta} = \binom{k+\beta-1}{k-1} = \Omega_{k,k,\beta,0,0}$.

(iv) If $k \leq 0$, then $G_{i,j,k,l} = kg_{i,j,k,l} = 0$ by definition, and analogously, for $K - k \leq 0$, $G_{I-i,J-j,K-k,L-l} = 0$. For $0 < k < K$, we prove (4.3.68) by complete induction on $I + J$.

Both sides are 0 if $I + J < 0$, which provides the basis of induction. Assume that (4.3.68) holds when $I + J < M$. For $I + J = M$, start from

$$\sum_{i,j,l\geq 0} H_{i,j,k,l}\odot H_{I-i,J-j,K-k,L-l} \tag{4.3.72}$$

and use (4.3.66) to replace $H_{i,j,k,l}$ and $H_{I-i,J-j,K-k,L-l}$. That gives four sums, one of terms of the form $\Xi\odot\Xi$, two of the form $\Xi\odot\Omega\odot G$ and one of the form $\Omega\odot\Omega\odot G\odot G$. Use (4.3.69) to compute the sum of $\Xi\odot\Xi$, use (4.3.71) to replace the sums of $\Xi\odot\Omega\odot G$ by sums of $\Omega\odot\Omega\odot G$, and use the inductive assumption to replace the sum of $\Omega\odot\Omega\odot G\odot G$ by a sum of $\Omega\odot\Omega\odot G$ (this will be possible for all terms except $\Omega_{K-k,0,0,0,0}\odot\Omega_{k,0,0,0,0}\odot G_{I,J,K,L}$ because for that term $I+J$ is not less than M). Finally, using (4.3.70) to replace the sum of $\Omega\odot\Omega\odot G$ by a sum of $\Omega\odot G$ and using (4.3.67) to combine terms, we conclude that (4.3.72) is equal to

$$H_{I,J,K,L}-G_{I,J,K,L}+\sum_{i,j,l\geq 0}G_{i,j,k,l}\odot G_{I-i,J-j,K-k,L-l} \tag{4.3.73}$$

However, applying (4.3.67) to $H_{I,J,K,L}$, $H_{i,j,k,l}$, $H_{I-i,J-j,K-k,L-l}$, one gets

$$\frac{\sum_{i,j,l\geq 0}H_{i,j,k,l}\odot H_{I-i,J-j,K-k,L-l}}{\sum_{i,j,l\geq 0}G_{i,j,k,l}\odot G_{I-i,J-j,K-k,L-l}}=\frac{H_{I,J,K,L}}{G_{I,J,K,L}} \tag{4.3.74}$$

From (4.3.72)=(4.3.73) and (4.3.74), we conclude that (4.3.68) holds for our choice of I,J,K,L, which completes the inductive step.

We prove (v) and (vi) simultaneously by induction on $I+J$.

If (vi) holds for $I+J<M$: by (4.3.55), singularities of $f_{I,J,K,L}$ come from a $g_{i,j,k,l}$ with $i+j<I+J$, so (v) then holds for $I+J\leq M$.

If (v) holds for $I+J<M$: by applying (4.3.68) $K-1$ times, $g_{I,J,K,L}$ can be written as a sum of K-fold products of $g_{i,j,1,l}$ with $i+j\leq I+J$. Thus, all its nonremovable singularities are singularities of a $g_{i,j,1,l}$ with $i+j\leq I+J$. By (4.3.52), those can only be of the form (4.3.43) with $k=1$ or coming from $f_{i,j,1,l}$. Thus, (vi) holds for $I+J\leq M$.

For (vii) and (viii), note that in the $L=0$ case (4.3.55) becomes

$$f_{I,J,K,0}=\xi_{I,J,K,0}+\sum_{\substack{\alpha,\gamma\geq 0\\ \alpha+\gamma\geq 1}}\omega_{K,\alpha,0,\gamma,0}\odot g_{I-\alpha,J-\gamma,K+\gamma-\alpha,0} \tag{4.3.75}$$

where $\xi_{I,J,K,0}=\delta_{I-K}\delta_J$. Induction on (4.3.75) using (4.3.52) then shows that $f_{I,J,K,0}=g_{I,J,K,0}=0$ unless $I-J=K$. With this observation in mind, the proof of (vii) and (viii) is analogous to the proof of (v) and (vi) above, using (4.3.75) instead of (4.3.55). □

For OPRL, if we are in the ℓ^p case, we encounter functions $f_{I,J,K,L}$ and $g_{I,J,K,L}$ with $I+J<p$. Lemma 4.3.5(v),(vi) implies that all of their nonremovable singularities are of the form (4.3.43) with $k=1$ and $i+j<p$. All such points are in the set A_p given by (4.3.12), so all iterations of Lemma 4.3.4 can be performed away from A_p.

For OPUC, since $c=0$, terms with $L>0$ vanish. For terms with $L=0$, Lemma 4.3.5(vii),(viii) implies that all nonremovable singularities of $f_{I,J,K,0}$ and $g_{I,J,K,0}$ are of the form (4.3.43) with $k = i - j = 1$ and $i + j < p$. All such points are in the set A_p given by (4.3.12), so all iterations of Lemma 4.3.4 can be performed away from A_p.

4.3.6 Proof in the general case

In this subsection, we complete the proofs of Theorems 4.2.1 and 4.2.2 in the general ℓ^p case. As hinted before, the key idea will be to use Lemma 4.3.3(ii); we will be able to prove that if $\log r_n$ didn't converge as desired, it would be possible to construct a set of recursion coefficients (corresponding to a measure) for which it diverged uniformly on an interval, contradicting Lemma 4.3.3(ii).

As explained in the previous section, the first step in the proof is to start with (4.3.48) and iteratively apply Lemma 4.3.4 to terms of the form

$$f_{I,J,K,L}\big(\eta; \{\phi_{k_i}\}_{i=1}^I; \{\phi_{l_j}\}_{j=1}^J\big) \prod_{i=1}^I (h_{k_i}(\eta)\beta_n^{(k_i)}) \prod_{j=1}^J (\bar{h}_{l_j}(\eta)\bar{\beta}_n^{(l_j)}) e^{iK[(n+1)\eta+2\theta_n]}\, c^L$$

in increasing order of $I + J$. In the previous section, we have seen that the only singularities we will encounter in these iterations are in A_p.

Lemma 4.3.4 can be applied to a term unless $K = 0$ and $\phi \in 2\pi\mathbb{Z}$, so after the iterative procedure, what remains is a sum of such terms,

$$\log \frac{r_{n+1}}{r_n} \sim_{A_p} \operatorname{Re} \sum \left(f_{I,J,0,L}\big(\eta; \{\phi_{k_i}\}_{i=1}^I; \{\phi_{l_j}\}_{j=1}^J\big) \prod_{i=1}^I (h_{k_i}(\eta)\beta_n^{(k_i)}) \prod_{j=1}^J (\bar{h}_{l_j}(\eta)\bar{\beta}_n^{(l_j)})\, c^L \right) \quad (4.3.76)$$

with the sum going over $(I + J)$-tuples $(k_1, \dots, k_I, l_1, \dots, l_J)$ with

$$\phi_{k_1} + \cdots + \phi_{k_I} - \phi_{l_1} - \cdots - \phi_{l_J} = 0 \quad (4.3.77)$$

and $I + J < p$.

At this point, a change of notation will be useful. Our proof in this section will rely on constructing counterexamples, and for that it would be useful to be able to construct $\beta^{(l)}$'s independently. For OPUC this is true, but for OPRL, by Lemma 4.3.2(vii), $\beta^{(l)}$'s come in complex-conjugate pairs: for every $\beta^{(l)}$ there is a $\beta^{(k)} = \bar{\beta}^{(l)}$. For each such pair, let us keep only one of the two sequences, say $\beta^{(l)}$, and replace $\beta^{(k)}$ everywhere by $\bar{\beta}^{(l)}$. This is equivalent to replacing (4.3.9) by

$$\alpha_n(\eta) = \sum_{l=1}^{L'} h_l(\eta)(\beta_n^{(l)} + c\bar{\beta}_n^{(l)}) \quad (4.3.78)$$

Notice that the right-hand side of (4.3.76) is the real part of a polynomial in $\beta_n^{(l)}$ and $\bar{\beta}_n^{(l)}$, with coefficients continuous in η. Denoting this polynomial by Q, (4.3.76) becomes

$$\log \frac{r_{n+1}}{r_n} \sim_{A_p} \operatorname{Re} Q(\eta; \beta_n^{(1)}, \dots, \beta_n^{(L)}; \bar{\beta}_n^{(1)}, \dots, \bar{\beta}_n^{(L)}) \tag{4.3.79}$$

We now make the claim that the right-hand side vanishes identically.

Lemma 4.3.6. *For all $\eta \notin A_p + 2\pi\mathbb{Z}$ and all $z_1, \dots, z_L \in \mathbb{C}$,*

$$\operatorname{Re} Q(\eta; z_1, \dots, z_L; \bar{z}_1, \dots, \bar{z}_L) = 0 \tag{4.3.80}$$

Proof. The proof will proceed by contradiction. Split Q into a sum of homogeneous polynomials $Q_1, \dots, Q_{p-1}$ with $\deg Q_k = k$. If the claim of the lemma is false, then there exists a smallest k such that $\operatorname{Re} Q_k$ does not vanish identically, and a choice of $\eta_0, z_1, \dots, z_L$ such that

$$\operatorname{Re} Q_k(\eta_0; z_1, \dots, z_L; \bar{z}_1, \dots, \bar{z}_L) \neq 0$$

Since Q depends only on the values of p, the phases $\phi_1, \dots, \phi_L$, and $h_1(\eta), \dots, h_L(\eta)$, but not on $\beta_n^{(l)}$, we are free to make a choice for $\beta_n^{(l)}$. Let

$$\beta_n^{(l)} = \begin{cases} z_l e^{-in\phi_l} n^{-1/(p-1)}, & \text{for } n \geq n_0 \\ 0, & \text{for } n < n_0 \end{cases} \tag{4.3.81}$$

Note that $\beta^{(l)} \in \ell^p \cap GBV(\phi_l)$. Through (4.3.78), this choice of $\beta^{(l)}$ corresponds to a sequence of recursion coefficients, if we choose n_0 large enough that the recursion coefficients are in the allowed range ($|\alpha_n| < 1$ for OPUC, $a_n^2 - 1 > -1$ for OPRL). By Verblunsky's or Stieltjes' theorem, (4.3.81) then corresponds to a probability measure on the unit circle or real line. Thus, (4.3.79) holds for the choice (4.3.81).

For every monomial $\beta_n^{(k_1)} \cdots \beta_n^{(k_I)} \bar{\beta}_n^{(l_1)} \cdots \bar{\beta}_n^{(l_J)}$ in Q, the condition (4.3.77) is satisfied, so the factors $e^{-in\phi_l}$ cancel out completely in Q, and substituting (4.3.81) into (4.3.79) gives

$$\log \frac{r_{n+1}}{r_n} \sim_{A_p} \sum_{l=1}^{p-1} \operatorname{Re} Q_l(\eta; z_1, \dots, z_L; \bar{z}_1, \dots, \bar{z}_L)\, n^{-l/(p-1)} \tag{4.3.82}$$

Summing (4.3.82) in n, the nonzero term with $l = k$ dominates the sum, and since the sum $\sum_{n=1}^{\infty} n^{-k/(p-1)}$ is divergent, this implies that $\log r_n$ converges to $+\infty$ or $-\infty$ (depending on the sign of $\operatorname{Re} Q_k$) uniformly in η on a neighborhood of η_0. By Lemma 4.3.3(ii), this is a contradiction, so (4.3.80) holds. □

By Lemma 4.3.6, (4.3.79) becomes (4.3.13). By Lemma 4.3.3(ii), this completes the proof of

Theorems 4.2.1 and 4.2.2.

4.4 Proof of Theorem 4.2.5

In this section, we will present the proof of Theorem 4.2.5. The proof relies on the same ideas seen in the previous section, and will go through similar steps, but will not rely on facts from that section.

We begin by discussing some relevant properties of functions of generalized bounded variation in Subsection 1. Subsection 2 will reduce the proof of the theorem to an iterative procedure, Subsection 3 will prove some functional identities, and Subsection 4 will complete the proof.

4.4.1 Functions of generalized bounded variation

In this section we describe some properties of functions of rotated and generalized bounded variation. In particular, we show that real functions of generalized bounded variation have, in essence, an even set of phases and a symmetric representation with respect to complex conjugation.

Lemma 4.4.1. *Let $\phi, \psi \in \mathbb{R}$, let $A, B, C \subset \mathbb{R}$ be finite sets, and $\beta(x)$, $\gamma(x)$ functions on $(0, \infty)$. Then*

(i) *If $\beta(x)$ has rotated bounded variation, then $\beta(x)$ is bounded.*

(ii) *If $\beta(x)$ and $\gamma(x)$ have rotated bounded variation with phases ϕ and ψ, respectively, then $\beta(x)\gamma(x)$ has rotated bounded variation with phase $\phi + \psi$.*

(iii) *If $\beta(x) \in GBV(B)$, $\gamma(x) \in GBV(C)$, then $\beta(x)\gamma(x) \in GBV(B + C)$.*

(iv) *If $\beta(x) \in GBV(B)$, $\gamma(x) \in GBV(C)$, then $\beta(x) + \gamma(x) \in GBV(B \cup C)$.*

(v) *If $\beta(x) \in GBV(B)$, then $\overline{\beta(x)} \in GBV(-B)$.*

Proof. For a function β of bounded variation, we will denote by $\mathcal{V}(\beta)$ its total variation,

$$\mathcal{V}(\beta) = \sup_{\substack{n \in \mathbb{N} \\ x_1 < x_2 < \cdots < x_n}} \sum_{k=1}^{n-1} |\beta(x_{k+1}) - \beta(x_k)| \tag{4.4.1}$$

It is a standard fact that functions of bounded variation are bounded, since for any x,

$$|\beta(x)| \leq |\beta(x_0)| + |\beta(x) - \beta(x_0)| \leq |\beta(x_0)| + \mathcal{V}(\beta)$$

This carries over trivially to functions of rotated bounded variation, proving (i).

For functions β, γ of bounded variation,

$$\begin{aligned}\left|\beta(y)\gamma(y)-\beta(x)\gamma(x)\right| &\le \left|\gamma(y)(\beta(y)-\beta(x))\right| + \left|\beta(x)(\gamma(y)-\gamma(x))\right| \\ &\le \|\gamma\|_\infty \left|\beta(y)-\beta(x)\right| + \|\beta\|_\infty \left|\gamma(y)-\gamma(x)\right|\end{aligned}$$

Applying this to $x = x_k$ and $y = x_{k+1}$ and using in combination with (4.4.1) gives

$$\mathcal{V}(\beta\gamma) \le \|\gamma\|_\infty \, \mathcal{V}(\beta) + \|\beta\|_\infty \, \mathcal{V}(\gamma)$$

The result extends trivially to sequences of rotated bounded variation, proving (ii).

(iii) follows from (ii) with the observation that products of a bounded sequence and an L^1 sequence are bounded.

(iv) and (v) follow directly from Definition 4.1.2. □

As a final bit of preparation, we remind the reader that our potential V has the decomposition (4.2.5), i.e.

$$V(x) = \sum_{l=1}^{L} \beta_l(x) + W(x) \tag{4.4.2}$$

where β_l has rotated bounded variation with phase $\phi_l \in A$, $\beta_l \in L^p$ for some $p \in [1,\infty)$, $\lim_{x\to\infty} \beta_l(x) = 0$, and $W \in L^1(1,\infty)$. It will be useful to make some adjustments to the breakup (4.4.2).

Since V is real-valued, by taking the average of (4.4.2) and its complex conjugate, we may assume that for any β_l in the sum (4.4.2), there is an β_k in the sum with $\bar{\beta}_k = \beta_l$.

It will be useful to adjust the breakup in (4.4.2) so that $\beta_l \in C^1$. That this is possible is an observation made by Weidmann [77] when proving Theorem 4.1.1. The proof we present is from Simon [58].

Lemma 4.4.2. *If $V(x)$ is of the form* (4.4.2)*, with β_l, W as described there, the breakup can be adjusted so that, in addition to assumptions stated there, $\beta_l \in C^1(1,\infty)$ and*

$$\frac{d}{dx}\left(e^{i\phi_l x}\beta_l(x)\right) \in L^1(1,\infty) \tag{4.4.3}$$

Proof. By linearity, it suffices to prove this fact for $L = 1$, and by multiplying by $e^{-i\phi_l x}$, it suffices to prove it when $\beta = \beta_1$ has bounded variation. Since every function of bounded variation is the linear combination of four bounded real-valued increasing functions, by linearity it suffices to prove it when β is an increasing function.

In addition, we extend β to a function on $\mathbb{R}$, with $\beta(y) = \lim_{x\downarrow 1} \beta(x)$ for $y \le 1$. Picking $j \in C_0^\infty(-1,1)$ with $j \ge 0$ and $\|j\|_1 = 1$, we define $\tilde{\beta} = j * \beta$. We will show that replacing β by $\tilde{\beta}$ in the decomposition (4.4.2) and absorbing $\beta - \tilde{\beta}$ into $W(x)$ fulfills all the requirements. Then by dominated convergence,

$$\lim_{y\to x}\frac{\tilde\beta(y)-\tilde\beta(x)}{y-x}=\int\frac{j(y-t)-j(x-t)}{y-x}\beta(t)dt=\int j'(x-t)\beta(t)dt=(j'*\beta)(x) \tag{4.4.4}$$

exists for all x so $\tilde\beta$ is differentiable. Moreover, since j is nonnegative and $\beta(x)$ is an increasing function, $\tilde\beta$ is also increasing and $\tilde\beta'\geq 0$. Since $\beta(x)$ has finite limits as $x\to\pm\infty$, dominated convergence implies

$$\lim_{x\to\pm\infty}\tilde\beta(x)=\lim_{x\to\pm\infty}\int_{-1}^{1}j(t)\beta(x-t)dt=\lim_{x\to\pm\infty}\beta(x)$$

which proves that $\tilde\beta'\in L^1$ with $\|\tilde\beta'\|_1=\beta(x)|_{-\infty}^{+\infty}=\mathcal{V}(\beta)$. If β is in L^p, then by Hölder's inequality,

$$|\tilde\beta(x)|^p\leq\left(\int_{-1}^{1}|j(t)\beta(x-t)|dt\right)^p\leq\left(\int_{-1}^{1}j(t)dt\right)^{p-1}\left(\int_{-1}^{1}j(t)|\beta(x-t)|^pdt\right)\leq\int_{-1}^{1}j(t)|\beta(x-t)|^pdt$$

so integrating in x, we see $\tilde\beta\in L^p$ with $\|\tilde\beta\|_p\leq\|\beta\|_p$.

Since β is increasing, it has an at most countable set B of points of discontinuity, and there exists a positive Stieltjes measure μ such that $\beta(x)=\mu([x,\infty))$ for $x\notin B$. Moreover, μ is finite and $\mu(\mathbb{R})=\mathcal{V}(\beta)$. Finally, for $x\notin B$, since $\operatorname{supp}j\subset[-1,1]$, $j\geq 0$, and $\|j\|_1=1$,

$$|\tilde\beta(x)-\beta(x)|=\big|(j*\beta)(x)-\mu([x,\infty))\big|\leq\int_{-1}^{1}j(t)\big|\mu([x-t,\infty))-\mu([x,\infty))\big|dt\leq\mu([x-1,x+1))$$

and integrating in x, since B is at most countable, we get $\tilde\beta-\beta\in L^1$ with $\|\tilde\beta-\beta\|_1\leq 2\mathcal{V}(\beta)$. $\square$

Note that by taking j with support in $[-\epsilon,\epsilon]$ instead of $[-1,1]$ in the previous proof, one can make $\tilde\beta-\beta$ arbitrarily small in L^1-norm. Moreover, by iterating the argument (4.4.4), one can conclude $\tilde\beta\in C^\infty$.

4.4.2 Reducing the proof to an iterative procedure

In this subsection, we reduce the problem to a criterion in terms of Prüfer variables (defined in Section 3.4), and establish a lemma that will be used iteratively in the proof.

For a given set of phases A, we will now define sets A_p for $p\in\mathbb{N}$. Let

$$A_p=\bigcup_{k=1}^{p-1}(\underbrace{A+\cdots+A}_{k\text{ times}}) \tag{4.4.5}$$

Since $A = -A$, the set A_p contains all elements of

$$(\underbrace{A + \cdots + A}_{i \text{ times}}) - (\underbrace{A + \cdots + A}_{j \text{ times}})$$

for any $i \geq 1$, $j \geq 0$ and $i + j < p$.

Definition 4.4.1. Let $B \subset (0, +\infty)$ be a finite set. We define a binary relation $\sim_B$ on the set of functions parametrized by $\eta \in (0, +\infty)$ by: $u_\eta(x) \sim_B v_\eta(x)$ if and only if

$$\lim_{M \to +\infty} \int_1^M \big(u_\eta(x) - v_\eta(x)\big)\, dx$$

converges uniformly (but not necessarily absolutely) in $\eta \in I$ for compact intervals $I \subset (0, +\infty)$ with $\operatorname{dist}(I, B) > 0$.

With this notation, if we are in the L^p case, our goal will be to show that for any initial condition $R_\eta(1) = R^{(0)} > 0$, $\theta_\eta(1) = \theta^{(0)} \in \mathbb{R}$,

$$\frac{d}{dx} \log R_\eta(x) \sim_{A_p} 0 \tag{4.4.6}$$

Denoting

$$S = \left\{ \frac{\eta^2}{4} \,\middle|\, \eta \in A_p \right\}$$

by Lemma 3.4.3, (4.4.6) implies absence of subordinate solutions for $E \in (0, \infty) \setminus S$ at infinity, so by Theorem 3.4.2, $\sigma_{\text{ac}}(H) \supset [0, +\infty)$ and $\sigma_{\text{s}}(H) \cap [0, \infty) \subset S$. Our Schrödinger operator restricted to $(0, 1)$ has no essential spectrum, and restricted to $(1, \infty)$ has essential spectrum $[0, \infty)$ by Theorem 3.3.6, so Theorem 3.4.2 implies that on $(0, \infty)$, $\sigma_{\text{ess}}(H) = [0, \infty)$, which then implies all the claims of Theorem 4.2.5.

The fact that convergence is uniform in η is actually not needed, but will come automatically with the proof. Even more, the proof below actually shows that convergence is uniform in initial conditions $R^{(0)}$ and $\theta^{(0)}$ as well.

In proving (4.4.6), we will rely on the two recurrence equations (3.4.12), (3.4.13), which we repeat for convenience:

$$\frac{d\theta_\eta}{dx} = -\frac{V(x)}{\eta} \Big(1 - e^{i[\eta x + 2\theta_\eta(x)]} - e^{-i[\eta x + 2\theta_\eta(x)]}\Big) \tag{4.4.7}$$

$$\frac{d}{dx} \log R_\eta(x) = \operatorname{Im}\Big(\frac{V(x)}{\eta} e^{i[\eta x + 2\theta_\eta(x)]}\Big) \tag{4.4.8}$$

Finally, V has the decomposition (4.4.2) and by Lemma 4.4.2, we assume that $\beta_l \in C^1$ and $\frac{d}{dx}\big(e^{i\phi_l x} \beta_l(x)\big) \in L^1$.

Comparing (4.4.6) and (4.4.8), we are motivated to find a way to control expressions of the form $f(\eta)\Gamma(x)e^{i[\eta x+2\theta_\eta(x)]}$. The following lemma will give us a way of passing from expressions of the form $f(\eta)\Gamma(x)e^{ik[\eta x+2\theta_\eta(x)]}$, $k \in \mathbb{Z}$, to expressions with faster decay at infinity, but at the cost of a multiplicative factor with a possible singularity in η. These singularities will correspond to elements of A_p, which our method will have to avoid. The main idea of the proof is that for η away from ϕ, the exponential factor $e^{i\phi x}$ in this function helps average out parts of it when integrals are taken.

Lemma 4.4.3. *Let $k \in \mathbb{Z}$ and $\phi \in \mathbb{R}$, with k and ϕ not both equal to 0. Let $B \subset \mathbb{R}$ be a finite set and $f\colon (0,+\infty)\setminus B \to \mathbb{C}$ be a continuous function such that*

$$g(\eta) = -2k\frac{f(\eta)}{k\eta-\phi} \tag{4.4.9}$$

is also continuous on $(0,+\infty)\setminus B$ (removable singularities in g are allowed).

(i) If $\Gamma \in L^1(1,\infty)$, then

$$f(\eta)\Gamma(x)e^{ki[\eta x+2\theta_\eta(x)]} \sim_B 0 \tag{4.4.10}$$

(ii) If $\Gamma \in C^1(1,\infty)$, $\frac{d}{dx}\left(e^{i\phi x}\Gamma(x)\right) \in L^1(1,\infty)$ and $\lim_{x\to\infty}\Gamma(x) = 0$, then

$$f(\eta)\Gamma(x)e^{ki[\eta x+2\theta_\eta(x)]} \sim_B g(\eta)\Gamma(x)e^{ki[\eta x+2\theta_\eta(x)]}\frac{d\theta_\eta}{dx} \tag{4.4.11}$$

It might seem extraneous to explicitly require that both f and g be continuous; however, we want the lemma to cover both the case $k \neq 0$, when f can be computed from (4.4.9) and is continuous if g is, and the case $k=0$, $\phi \neq 0$, when $g \equiv 0$ and we want to allow f to be any continuous function.

Proof. (i) Since $|e^{ki[\eta x+2\theta_\eta(x)]}| = 1$,

$$\lim_{M\to\infty}\int_1^M f(\eta)\Gamma(x)e^{ki[\eta x+2\theta_\eta(x)]}$$

exists by dominated convergence and convergence is uniform since f is bounded on compact subsets of $(0,+\infty)\setminus B$.

(ii) Let $\gamma(x) = e^{i\phi x}\Gamma(x)$ and $h(\eta) = f(\eta)/(k\eta-\phi)$. By the product rule,

$$\begin{aligned}\frac{d}{dx}\left[h(\eta)\gamma(x)e^{i[(k\eta-\phi)x+2k\theta_\eta(x)]}\right] &= h(\eta)\gamma'(x)e^{i[(k\eta-\phi)x+2k\theta_\eta(x)]} \\ &\quad + ih(\eta)\gamma(x)e^{i[(k\eta-\phi)x+2k\theta_\eta(x)]}\left[k\eta-\phi+2k\frac{d\theta_\eta}{dx}\right]\end{aligned} \tag{4.4.12}$$

Note that h is continuous on $(0,+\infty)\setminus B$, by continuity of g for $k \neq 0$ and by continuity of f for $k=0$ and $\phi \neq 0$. Thus, h is bounded on compact subsets of $(0,+\infty)\setminus B$ and together with $\lim_{x\to\infty}\gamma(x) = 0$, this implies that $h(\eta)\gamma(x)e^{i[(k\eta-\phi)x+2k\theta_\eta(x)]}$ converges to 0 uniformly in η away from B as $x \to \infty$.

Boundedness of h away from B together with $\gamma' \in L^1(1,\infty)$ implies

$$h(\eta)\gamma'(x)e^{i[(k\eta-\phi)x+2k\theta_\eta(x)]} \sim_B 0$$

Thus, taking the integral $\int_1^M dx$ of (4.4.12) and taking the limit as $M \to \infty$ gives

$$h(\eta)\gamma(x)e^{i[(k\eta-\phi)x+2k\theta_\eta(x)]}\Big[k\eta - \phi + 2k\frac{d\theta}{dx}\Big] \sim_B 0$$

which can be rewritten as (4.4.11) since $f(\eta) = (k\eta - \phi)h(\eta)$ and $g(\eta) = -2kh(\eta)$. □

We now present the proof in the L^2 case, as a warmup for the general case. By (4.4.8) and (4.4.2),

$$\begin{aligned}
\frac{d}{dx}\log R_\eta(x) &= \operatorname{Im}\Big(\frac{V(x)}{\eta}e^{i[\eta x+2\theta_\eta(x)]}\Big) \\
&= \frac{1}{\eta}\operatorname{Im}\Big(\sum_{l=1}^{L}\beta_l(x)e^{i[\eta x+2\theta_\eta(x)]} + W(x)e^{i[\eta x+2\theta_\eta(x)]}\Big) \\
&= \frac{1}{\eta}\operatorname{Im}\Big(-\sum_{l=1}^{L}\frac{2k}{\eta-\phi_l}\beta_l(x)e^{i[\eta x+2\theta_\eta(x)]}\frac{d\theta_\eta}{dx}\Big) \\
&= \frac{1}{\eta^2}\operatorname{Im}\Big(\sum_{l=1}^{L}\frac{2k}{\eta-\phi_l}\beta_l(x)V(x)e^{i[\eta x+2\theta_\eta(x)]}\big(1 - e^{i[\eta x+2\theta_\eta(x)]} - e^{-i[\eta x+2\theta_\eta(x)]}\big)\Big) \qquad (4.4.13)
\end{aligned}$$

where for the third line we applied Lemma 4.4.3 to each term separately and for the fourth we used (4.4.7). Using (4.4.2) again, we see that the right-hand side is a finite sum of two kinds of terms: those with $\beta_l(x)W(x)$ and those with $\beta_l(x)\beta_k(x)$. Since β_l is bounded, $\beta_l(x)W(x) \in L^1(1,\infty)$, and since $\beta_l, \beta_k \in L^2$, $\beta_l\beta_k \in L^1(1,\infty)$. Also note that the factors in η are continuous away from the ϕ_l. Thus, by Lemma 4.4.3(i),

$$\begin{aligned}
&\frac{1}{\eta^2}\frac{2k}{\eta-\phi_l}\beta_l(x)W(x)e^{i[\eta x+2\theta_\eta(x)]}\big(1 - e^{i[\eta x+2\theta_\eta(x)]} - e^{-i[\eta x+2\theta_\eta(x)]}\big)\Big) \sim_A 0 \\
&\frac{1}{\eta^2}\frac{2k}{\eta-\phi_l}\beta_l(x)\beta_k(x)e^{i[\eta x+2\theta_\eta(x)]}\big(1 - e^{i[\eta x+2\theta_\eta(x)]} - e^{-i[\eta x+2\theta_\eta(x)]}\big)\Big) \sim_A 0
\end{aligned}$$

and summing those into (4.4.13) proves (4.4.6), as desired.

The proof above worked because we were able to replace terms with β_l by terms with $\beta_l W$ and $\beta_l\beta_k$, at which point we could use the L^2 condition to control $\beta_l\beta_k$. To go beyond L^2, we will need to apply Lemma 4.4.3 iteratively, until we get products of p of the β_k's. After every application of Lemma 4.4.3, all the terms containing W will be L^1 and so $\sim_{A_p} 0$, and we will be left with terms with products of β_k's, with one more β than we started with. Using also the form of (4.4.7), we notice that we will only have terms of the form

$$f_{I,K}(\eta;\phi_{j_1},\ldots,\phi_{j_I})\beta_{j_1}(x)\ldots\beta_{j_I}(x)e^{i[K\eta x+2K\theta_\eta(x)]} \tag{4.4.14}$$

with $I \geq 1$, $0 \leq K \leq I$. Since terms of this form will occur with all permutations of $j_1,\ldots,j_I$, we can agree to average in all of those terms, so that $f_{I,K}$ will be periodic in $\phi_{j_1},\ldots,\phi_{j_I}$.

When we apply Lemma 4.4.3(ii) to such a term, the appropriate $g_{I,K}$ will be

$$g_{I,K}(\eta;\{\phi_i\}_{i=1}^I) = -\frac{2K}{K\eta - \sum_{i=1}^I \phi_i} f_{I,K}(\eta;\{\phi_i\}_{i=1}^I) \tag{4.4.15}$$

From (4.4.8) we read off

$$f_{1,K}(\eta;\phi_1) = \frac{\delta_{K-1}}{\eta}, \quad I = 1 \tag{4.4.16}$$

and by writing out which $g_{I-1,k}$ affect $f_{I,K}$ and remembering our convention to symmetrize in the ϕ_j, we obtain a recurrence relation in $f_{I,K}$ and $g_{I,K}$,

$$f_{I,K}(\eta;\{\phi_i\}_{i=1}^I) = \frac{1}{\eta}\sum_{k=K-1}^{K+1}\sum_{\sigma\in S_I}(-1)^{K-k-1}g_{I-1,k}(\eta;\{\phi_{\sigma(i)}\}_{i=1}^{I-1}), \quad I \geq 2 \tag{4.4.17}$$

There is one issue we haven't yet addressed: Lemma 4.4.3(ii) only applies when k and ϕ aren't both equal to 0. In our notation, this issue arises for terms

$$f_{I,0}(\eta;\phi_{j_1},\ldots,\phi_{j_I})\beta_{j_1}(x)\ldots\beta_{j_I}(x)$$

with $\phi_{j_1}+\cdots+\phi_{j_I} = 0$. We will need a separate argument to eliminate these terms, and this will come from a symmetry property of $f_{I,0}$ proved in the next subsection.

Finally, we wish to prove that all iterations of Lemma 4.4.3(ii) can be performed with $B = A_p$, and for that we need to be able to control the singularities of $g_{I,K}$. This will come from a functional identity in terms of the $g_{I,K}$, also proved in the next subsection.

4.4.3 Some functional identities

In this subsection, we will establish some properties of the functions $f_{I,K}$ and $g_{I,K}$, which will be used to restrict the set of their nonremovable singularities and to prove the vanishing of terms which Lemma 4.4.3 wouldn't be able to handle.

We begin by establishing the notation. We will be dealing with functions of $1+n$ variables, where the first variable will be η and the remaining n will be phases. In applications these will be some of the phases of generalized bounded variation, but in this subsection we think of them merely as parameters of certain functions. We need a kind of symmetrized product for such functions:

Definition 4.4.2. For a function p_I of $1+I$ variables and a function q_J of $1+J$ variables, we define their symmetric product as a function $p_I \odot q_J$ of $1+(I+J)$ variables by

$$(p_I \odot q_J)\big(\eta; \{\phi_i\}_{i=1}^{I+J}\big) = \frac{1}{(I+J)!} \sum_{\sigma \in S_{I+J}} p_I\big(\eta; \{\phi_{\sigma(i)}\}_{i=1}^{I}\big) q_J\big(\eta; \{\phi_{\sigma(i)}\}_{i=I+1}^{I+J}\big)$$

where S_{I+J} is the symmetric group in $I+J$ elements.

It is straightforward to see that $\odot$ is commutative and associative. We will also have a use for some auxiliary functions. Let Ω_a, with $a \in \mathbb{Z}$, be a function of $1+1$ variables and let $\Xi_{I,K}$, for $0 \le K \le I$, be a function of $1+I$ variables,

$$\Omega_a(\eta; \phi_1) = \begin{cases} 1, & a \in \{-1, 0, 1\} \\ 0, & \text{otherwise} \end{cases} \tag{4.4.18}$$

$$\Xi_{I,K}(\eta; \{\phi_k\}_{k=1}^{K}) = \delta_{I-1}\delta_{K-1} \tag{4.4.19}$$

These functions are, of course, constant but defining them as functions will be convenient for use with the symmetrized product. We will also introduce rescaled versions of the $f_{I,K}$ and $g_{I,K}$; for $I \ge 1$ and $0 \le K \le I$,

$$F_{I,K} = (-1)^{I-K} \frac{\eta^I}{(-2)^{I-1}} f_{I,K} \tag{4.4.20}$$

$$G_{I,K} = (-1)^{I-K} \frac{\eta^I}{(-2)^{I}} g_{I,K} \tag{4.4.21}$$

We will also take the convention

$$F_{0,0} = G_{0,0} = 0 \tag{4.4.22}$$

Rescaling (4.4.15), (4.4.16) and (4.4.17) gives

$$F_{I,K} = \Xi_{I,K} + \sum_{a=-1}^{1} \Omega_a \odot G_{I-1,K+a} \tag{4.4.23}$$

$$G_{I,K}(\eta; \{\phi_i\}_{i=1}^{I}) = \frac{K}{K\eta - \sum_{i=1}^{I} \phi_i} F_{I,K}(\eta; \{\phi_i\}_{i=1}^{I}) \tag{4.4.24}$$

Note that $F_{I,K}$ and $G_{I,K}$ have singularities, which makes us cautious about performing arithmetic with them. Note, however, that (4.4.23) and (4.4.24) define functions for complex values of all parameters, and that these functions are meromorphic in all parameters. Moreover, by (4.4.23) and (4.4.24), $F_{I,K}$ and $G_{I,K}$ can only have singularities for parameters $\eta, \{\phi_i\}_{i=1}^{I}$ such that $k\eta = \sum_{i \in A} \phi_i$ for some $0 < k < K$ and some $A \subset \{1, \ldots, I\}$, which is only a finite set of hyperplanes in $\mathbb{C}^{1+I}$. Thus, when proving identities like the ones that follow, we can perform the calculations for the case when all quantities are finite, and then extend by meromorphicity.

Lemma 4.4.4. (i) *For $0 \leq K \leq I$ and $0 < k < K$, the identities*

$$F_{I,K} = \sum_{i=0}^{I} F_{i,k} \odot G_{I-i,K-k} \tag{4.4.25}$$

$$G_{I,K} = \sum_{i=0}^{I} G_{i,k} \odot G_{I-i,K-k} \tag{4.4.26}$$

hold for all values of parameters for which all terms occurring in both sides are finite; if seen as equalities involving meromorphic functions, they hold identically.

(ii) *If*

$$\phi_1 + \cdots + \phi_I = 0 \tag{4.4.27}$$

then

$$F_{I,0}(\eta, \phi_1, \ldots, \phi_I) = F_{I,0}(\eta, -\phi_1, \ldots, -\phi_I) \tag{4.4.28}$$

(iii) *Nonremovable singularities of $F_{I,K}$ and $f_{I,K}$ for $\eta > 0$ are of the form*

$$\eta = \sum_{a=1}^{b} \phi_{m_a} \tag{4.4.29}$$

with $b < I$.

(iv) *Nonremovable singularities of $G_{I,K}$ and $g_{I,K}$ for $\eta > 0$ are of the form* (4.4.29) *with $b \leq I$.*

Proof. (i) We prove (4.4.25) and (4.4.26) simultaneously by induction on I. The statement is vacuous for $I \leq 1$. Assume it holds for $I - 1$. Then by (4.4.23),

$$\sum_{i=0}^{I} F_{i,k} \odot G_{I-i,K-k} = \sum_{i=0}^{I} (\Xi_{i,k} + \sum_{a=-1}^{1} \Omega_a \odot G_{i-1,k+a}) \odot G_{I-i,K-k}$$

Using the inductive assumption, we may apply (4.4.26) to the sums of $G \odot G$, unless $k + a \leq 0$. But $k + a \leq 0$ holds only for $k = 1$, $a = -1$, and in this exceptional case $G_{i-1,k+a} = 0$. Thus,

$$\begin{aligned}
\sum_{i=0}^{I} F_{i,k} \odot G_{I-i,K-k} &= \sum_{i=0}^{I} \Xi_{i,k} \odot G_{I-i,K-k} + \sum_{a=-1}^{1} \sum_{i=0}^{I} \Omega_a \odot G_{i-1,k+a} \odot G_{I-i,K-k} \\
&= \delta_{k-1} \Xi_{1,1} \odot G_{I-1,K-1} + \sum_{a=-1}^{1} \Omega_a \odot (G_{I-1,K+a} - \delta_{a+1}\delta_{k-1} G_{I-1,K-1}) \\
&= \delta_{k-1} \Xi_{1,1} \odot G_{I-1,K-1} + F_{I,K} - \Xi_{I,K} - \Omega_{-1}\delta_{k-1} G_{I-1,K-1} \\
&= F_{I,K}
\end{aligned}$$

where we used (4.4.23) in the third line and $\Xi_{1,1} = \Omega_{-1}$ and $\Xi_{I,K} = 0$ (since $I \geq 2$) in the fourth. We have thus proved part of the inductive step, proving that (4.4.25) holds for our value of I. It remains to prove (4.4.26).

For any permutation $\sigma \in S_I$, by (4.4.24),

$$G_{i,k}(\eta; \{\phi_{\sigma(j)}\}_{j=1}^{i}) = \frac{1}{k}\Big(k\eta - \sum_{j=1}^{i} \phi_{\sigma(j)}\Big) F_{i,k}(\eta; \{\phi_{\sigma(j)}\}_{j=1}^{i})$$

Multiplying by $G_{I-i,K-k}(\eta; \{\phi_{\sigma(j)}\}_{j=i+1}^{I})$ and averaging in all permutations σ, we get

$$G_{i,k} \odot G_{I-i,K-k} = \Big(\eta - \frac{1}{K}\sum_{j=1}^{I} \phi_j\Big) F_{i,k} \odot G_{I-i,K-k} \tag{4.4.30}$$

Taking the sum $\sum_{i=0}^{I}$ of (4.4.30) and using (4.4.25), we have

$$\sum_{i=0}^{I} G_{i,k} \odot G_{I-i,K-k} = \Big(\eta - \frac{1}{K}\sum_{j=1}^{I} \phi_j\Big) F_{I,K}$$

which, by (4.4.24), implies (4.4.26).

(ii) This identity will be obvious when written in the right way, but the notation is cumbersome. Let A_I be the set of sequences $\overrightarrow{k} = (k_0, k_1, \ldots, k_I)$ with $|k_i - k_{i+1}| \leq 1$, $k_i \geq 1$ for $0 < i < I$ and $k_0 = k_I = 0$, and let $H_{I,\overrightarrow{k}}$ be a function of $1 + I$ variables given by

$$H_{I,\overrightarrow{k},\sigma}(\eta; \phi_1, \ldots, \phi_I) = \prod_{i=1}^{I-1} \frac{k_i}{k_i\eta - \sum_{a=1}^{i} \phi_{\sigma(a)}} \tag{4.4.31}$$

This quantity is useful because, by a simple induction using (4.4.23) and (4.4.24),

$$F_{I,0} = \frac{1}{I!} \sum_{\sigma \in S_I} \sum_{\overrightarrow{k} \in A_I} H_{I,\overrightarrow{k},\sigma} \tag{4.4.32}$$

Now note that if $\overrightarrow{k}' = (k_I, k_{I-1}, \ldots, k_0)$ and σ' is the "reversed" permutation from σ defined by $\sigma'(j) = I + 1 - \sigma(I + 1 - j)$, then when (4.4.27) holds, we have

$$\frac{k_i'}{k_i'\eta + \sum_{j=1}^{i} \phi_{\sigma'(j)}} = \frac{k_{I-i}}{k_{I-i}\eta - \sum_{j=1}^{I-i} \phi_{\sigma(j)}}$$

Taking the product $\prod_{i=1}^{I-1}$ of this,

$$H_{I,\overrightarrow{k},\sigma}(\eta; \phi_1, \ldots, \phi_I) = H_{I,\overrightarrow{k}',\sigma'}(\eta; -\phi_1, \ldots, -\phi_I) \tag{4.4.33}$$

Summing in $\overrightarrow{k}$ and σ and using (4.4.32) proves (4.4.28).

(iii), (iv) We prove (iii) and (iv) simultaneously by induction on I.

If (iv) holds for $I < M$: by (4.4.23), singularities of $F_{I,K}$ come from a $G_{I-1,k}$, so (iii) then holds for $I \leq M$.

If (iii) holds for $I < M$: by applying (4.4.26) $K-1$ times, $G_{I,K}$ can be written as a sum of K-fold products of $G_{i,1}$ with $i \leq I$, so all its nonremovable singularities are singularities of a $G_{i,1}$ with $i \leq I$. By (4.4.24), those can only be of the form (4.4.29) with $b = i \leq I$, or coming from $f_{i,1}$, so again of that form with $b < i \leq I$. Thus, (iv) holds for $I \leq M$.

The statements for $f_{I,K}$ and $g_{I,K}$ follow from (4.4.20) and (4.4.21). □

4.4.4 Completing the proof

As described in Subsection 4.4.2, the proof will rely on an iterative process. We want to control $\frac{d}{dx} \log R_\eta(x)$, and because of (4.4.8), we start with

$$\frac{V(x)}{\eta} e^{i[\eta x + 2\theta_\eta(x)]} \tag{4.4.34}$$

which is a finite sum of terms of the form

$$f_{I,K}(\eta; \phi_{j_1}, \ldots, \phi_{j_I}) \beta_{j_1}(x) \ldots \beta_{j_I}(x) e^{i[K\eta x + 2K\theta_\eta(x)]} \tag{4.4.35}$$

We then use Lemma 4.4.3(ii) to replace terms (4.4.35) by finite sums of terms of the same form, but with a greater value of I. We proceed with this process until we get terms with $I \geq p$; and by Lemma 4.4.4(iv), all terms with $I < p$ will have their corresponding $g_{I,K}$ continuous (and thus bounded) away from the set A_p. Terms (4.4.35) with $I \geq p$ are in L^1, so they are negligible in the relation $\sim_{A_p}$.

Thus, the only terms we will be left with are the ones for which Lemma 4.4.3(ii) does not apply. These are terms with $K = 0$ and $\phi_{j_1} + \cdots + \phi_{j_I} = 0$. However, for any such term

$$f_{I,0}(\eta; \phi_{j_1}, \ldots, \phi_{j_I}) \beta_{j_1}(x) \ldots \beta_{j_I}(x) \tag{4.4.36}$$

in the sum, there is a corresponding term

$$f_{I,0}(\eta; -\phi_{j_1}, \ldots, -\phi_{j_I}) \bar{\beta}_{j_1}(x) \ldots \bar{\beta}_{j_I}(x) \tag{4.4.37}$$

because we have chosen a decomposition (4.4.2) of V such that for every β_i, there is a $\bar{\beta}_i$ in the decomposition. However, by Lemma 4.4.4(ii), the sum of (4.4.36) and (4.4.37) is purely real! Thus, when we take the imaginary part of (4.4.34), by (4.4.8) we get

$$\frac{d}{dx} \log R_\eta(x) \sim_{A_p} 0$$

which completes the proof.

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